L11 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2002:97692 CAPLUS Full-text

DN 137:103383

TI Synthesis and SAR of N-substituted dibenzazepinone derivatives as novel potent and selective  $\alpha V\beta 3$  antagonists

AU Kling, Andreas; Backfisch, Gisela; Delzer, Jurgen; Geneste, Herve; Graef, Claudia; Holzenkamp, Uta; Hornberger, Wilfried; Lange, Udo E. W.; Lauterbach, Arnulf; Mack, Helmut; Seitz, Werner; Subkowski, Thomas

CS Knoll GmbH, Ludwigshafen, D-67008, Germany

SO Bioorganic & Medicinal Chemistry Letters (2002), 12(3), 441-446 CODEN: BMCLE8; ISSN: 0960-894X

PB Elsevier Science Ltd.

DT Journal

LA English

OS CASREACT 137:103383

GΙ

Substituted oxodibenzazepineacetic acids substituted with guanidines or guanidine pharmacophores such as I are prepared as potential  $\alpha V\beta 3$  (vitronectin receptor) antagonists. The oxodibenzazepineacetic acid core II is prepared in 5 steps from 9,10-anthraquinone; coupling of II with guanidine or guanidine pharmacophore-substituted amines such as III followed by hydrolysis of the Me ester yields compds. such as I. Structure-activity relationships are determined for the guanidine or guanidine pharmacophore-substituted oxodibenzazepineacetic acids, varying the linker between the guanidine pharmacophore and the oxodibenzazepine and the choice of guanidine pharmacophore. Compound I and a second guanidine pharmacophore-substituted oxodibenzazepineacetic acid are found to be highly active inhibitors of the vitronectin receptor in vitro and are found to be bioavailable in ADME assays.

IT 326401-69-8P 326401-92-7P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation of a guanidine or guanidine pharmacophore-substituted oxodibenzazepineacetic acid and lack of activity as a potential  $\alpha V\beta 3$  receptor antagonist)

RN 326401-69-8 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[[4-

[(1-oxo-3-phenylpropyl)amino]phenyl]methyl]amino]ethyl]- (9CI) (CA

INDEX

NAME)

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Сн2-со2н

RN 326401-92-7 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-[[4-[[(phenylmethyl)amino]carbonyl]amino]phenyl]methoxy]ethyl]- (9CI) (CA INDEX NAME)

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Сн2-со2н

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326399-78-4P 326399-83-1P 326400-55-9P 326400-65-1P 326400-70-8P 326401-04-1P 326401-08-5P 326401-18-7P 326401-26-7P 326401-36-9P 326401-41-6P 326401-74-5P 326401-97-2P
```

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation of guanidine or guanidine pharmacophore-substituted oxodibenzazepineacetic acids as potential  $\alpha V\beta 3$  receptor antagonists)

RN 326398-90-7 CAPLUS

CN 35H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[6-(1H-benzimidazol-2-yl)-

pyridinyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo- (9CI) (CA INDEX NAME)

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. Сн<sub>2</sub> — со<sub>2</sub>н

326399-52-4 CAPLUS

RN

2-

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[5-(1H-benzimidazol-2-yl)-

thienyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo- (9CI) (CA INDEX NAME)

RN 326399-69-3 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-5-[2-[[[4-(1H-imidazo[4,5-b]pyridin-2-yl)-2-thienyl]methyl]amino]-2-oxoethyl]-6-oxo-(9CI) (CA INDEX NAME)

'RN 326399-78-4 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[4-(1H-benzimidazol-2-yl)-

2thiazolyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo- (9CI) (CA INDEX NAME)

RN 326399-83-1 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[4-(1H-benzimidazol-2-yl)phenyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo-(9CI) (CA INDEX NAME)

RN 326400-55-9 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[4-(1H-benzimidazol-2-ylamino)phenyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo- (9CI) (CA INDEX NAME)

RN 326400-65-1 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[5-(1H-benzimidazol-2-ylamino)pentyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo- (9CI) (CA INDEX NAME)

RN 326400-70-8 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[4-(1H-benzimidazol-2-

ylamino)butyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo- (9CI) (CA INDEX NAME)

RN 326401-04-1 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[2-[4-(1H-benzimidazol-2-yl)phenyl]ethyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo- (9CI) (CA INDEX NAME)

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 $c_{\rm H_2-co_2H}$ 

RN 326401-36-9 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[4-(5-chloro-1H-benzimidazol-2-yl)phenyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo-(9CI) (CA INDEX NAME)

 $L_{\text{CH}2-\text{CO}2\text{H}}$ 

RN 326401-41-6 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[4-(5,6-dimethyl-1H-benzimidazol-2-yl)phenyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo-(9CI) (CA INDEX NAME)

PAGE 1-A

Сн2-со2н

RN 326401-74-5 CAPLUS

CN 5H-Dibenz[b,e] azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[[4-oxo-2-1]]]

[[(phenylmethoxy)carbonyl]amino]phenyl]methyl]amino]ethyl]- (9CI) (CA INDEX NAME)

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Сн<sub>2</sub>— со<sub>2</sub>н

RN 326401-97-2 CAPLUS

CN

5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[4-[4-[[([(phenylmethyl)amino]carbonyl]amino]phenyl]butyl]- (9CI) (CA INDEX NAME)

## IT 90664-75-8

RL: RCT (Reactant); RACT (Reactant or reagent) (preparation of guanidine or guanidine pharmacophore-substituted oxodibenzazepineacetic acids as potential  $\alpha V\beta 3$  receptor antagonists)

RN 90664-75-8 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-, methyl ester (9CI) (CA INDEX NAME)

## IT 90664-74-7P 326400-60-6P 326401-22-3P 326404-40-4P 326404-44-8P 326404-49-3P 326408-08-6P 326408-33-7P 326410-52-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

(preparation of guanidine or guanidine pharmacophore-substituted oxodibenzazepineacetic acids as potential  $\alpha V\beta 3$  receptor antagonists)

RN 90664-74-7 CAPLUS

CN Acetic acid, (5,6-dihydro-6-oxo-11H-dibenz[b,e]azepin-11-ylidene)-, methyl

ester (9CI) (CA INDEX NAME)

RN 326400-60-6 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[4-(1H-benzimidazol-2-ylamino)phenyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo-, methyl ester

(9CI) (CA INDEX NAME)

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[[[4-

 $\label{lem:carbonyl} \begin{tabular}{l} [\ [\ (phenylmethyl)\ amino\ ]\ carbonyl\ ]\ amino\ ]\ phenyl\ ]\ methyl\ ]\ -, \\ methyl\ \\ \end{tabular}$ 

ester (9CI) (CA INDEX NAME)

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RN 326404-40-4 CAPLUS

CN 5H-Dibenz[b,e]azepine-5-acetic acid, 6,11-dihydro-11-(2-methoxy-2-oxoethylidene)-6-oxo-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{CH}_2-\text{C} & \text{OBu-t} \\ \hline \\ \text{CH}-\text{C}-\text{OMe} \\ \hline \\ \end{array}$$

RN 326404-44-8 CAPLUS

CN 5H-Dibenz[b,e]azepine-5,11-diacetic acid, 6,11-dihydro-6-oxo-,  $\alpha$ 5-(1,1-dimethylethyl)  $\alpha$ 11-methyl ester (9CI) (CA INDEX NAME)

RN 326404-49-3 CAPLUS

CN 5H-Dibenz[b,e]azepine-5,11-diacetic acid, 6,11-dihydro-6-oxo-,  $\alpha$ 11-methyl ester (9CI) (CA INDEX NAME)

RN

326408-08-6 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[6-(1H-benzimidazol-2-yl)-3-]

pyridinyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo-, methyl ester
(9CI) (CA INDEX NAME)

RN 326408-33-7 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[4-(1H-benzimidazol-2-yl)-2thienyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo-, methyl ester
(9CI)
(CA INDEX NAME)

RN 326410-52-0 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-5-(2-hydroxyethyl)-6-oxo-, methyl ester (9CI) (CA INDEX NAME)

RE.CNT 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L11 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2005 ACS on STN
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AN 2001:115130 CAPLUS Full-text

DN 134:178474

TI Preparation of oxobenzazepinealkanoates and analogs as integrin receptor antagonists

IN Kling, Andreas; Geneste, Herve; Lange, Udo; Lauterbach, Arnulf; Graef, Claudia Isabella; Subkowski, Thomas; Holzenkamp, Uta; Mack, Helmut; Sadowski, Jens; Hornberger, Wilfried; Laux, Volker

PA BASF Aktiengesellschaft, Germany

SO PCT Int. Appl., 158 pp.

CODEN: PIXXD2

DT Patent

LA German

FAN.CNT 1

| E MIN • | PATENT NO.       |                          |                                 |                                 |                                 | KIND                            |                                 | DATE                            |      | APPLICATION NO.          |                          |                          |                          |                          | DATE              |                   |                   |            |  |
|---------|------------------|--------------------------|---------------------------------|---------------------------------|---------------------------------|---------------------------------|---------------------------------|---------------------------------|------|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|-------------------|-------------------|-------------------|------------|--|
| ΡI      |                  | 2001010847<br>2001010847 |                                 |                                 |                                 |                                 |                                 |                                 |      | WO 2000-EP7440           |                          |                          |                          |                          |                   | 20000801          |                   |            |  |
|         |                  |                          | AE,<br>CR,<br>HU,<br>LU,<br>SD, | AG,<br>CU,<br>ID,<br>LV,<br>SE, | AL,<br>CZ,<br>IL,<br>MA,<br>SG, | AM,<br>DE,<br>IN,<br>MD,<br>SI, | AT,<br>DK,<br>IS,<br>MG,<br>SK, | AU,<br>DM,<br>JP,<br>MK,<br>SL, |      | EE,<br>KG,<br>MW,<br>TM, | ES,<br>KP,<br>MX,<br>TR, | FI,<br>KR,<br>MZ,<br>TT, | GB,<br>KZ,<br>NO,<br>TZ, | GD,<br>LC,<br>NZ,<br>UA, | GE,<br>LK,<br>PL, | GH,<br>LR,<br>PT, | GM,<br>LS,<br>RO, | LT,<br>RU, |  |
|         |                  | RW:                      | GH,<br>DE,                      | GM,<br>DK,                      | KE,<br>ES,                      | LS,<br>FI,                      | MW,<br>FR,                      | ΜΖ,<br>GB,                      | •    | SL,<br>IE,               | SZ,<br>IT,               | TZ,<br>LU,               | UG,<br>MC,               | ZW,<br>NL,               | PT,               |                   |                   | CY,<br>BJ, |  |
|         | DE               | E 19936780               |                                 |                                 |                                 |                                 |                                 |                                 |      | DE 1999-19936780         |                          |                          |                          |                          | 19990809          |                   |                   |            |  |
|         | CA               |                          |                                 |                                 |                                 |                                 |                                 |                                 |      | CA 2000-2379977          |                          |                          |                          |                          |                   | 20000801          |                   |            |  |
|         | ΕP               | 1202988                  |                                 |                                 | EP 2000-958347                  |                                 |                                 |                                 |      |                          |                          |                          |                          |                          |                   |                   |                   |            |  |
|         |                  | R:                       | AT,                             | BE,                             | CH,                             | DE,                             | DK,                             | ES,                             | FR,  | GB,                      | GR,                      | IT,                      | LI,                      | LU,                      | NL,               | SE,               | MC,               | PT,        |  |
|         |                  |                          | IE,                             | SI,                             | LT,                             | LV,                             | FI,                             | RO,                             | MK,  | CY,                      | AL                       |                          |                          |                          |                   |                   |                   |            |  |
|         | BR               | R 2000013265             |                                 |                                 |                                 |                                 | 20020514                        |                                 |      | BR 2000-13265            |                          |                          |                          |                          |                   | 20000801          |                   |            |  |
|         | TR               | 'R 200200357             |                                 |                                 |                                 |                                 |                                 | 2002                            | 0923 | TR 2002-200200357        |                          |                          |                          |                          |                   | 20000801          |                   |            |  |
|         |                  | JP 2003506441            |                                 |                                 |                                 |                                 |                                 | 20030218                        |      |                          | JP 2001-515313           |                          |                          |                          |                   |                   | 20000801          |            |  |
|         |                  | 3G 106395                |                                 |                                 |                                 |                                 |                                 |                                 |      | BG 2002-106395           |                          |                          |                          |                          |                   |                   |                   |            |  |
|         |                  | NO 2002000644            |                                 |                                 |                                 |                                 |                                 |                                 |      |                          | NO 2002-644              |                          |                          |                          |                   |                   | 20020208          |            |  |
| PRAI    | DE 1999-19936780 |                          |                                 |                                 |                                 |                                 |                                 | 1999                            |      |                          |                          |                          |                          |                          |                   |                   |                   |            |  |
|         |                  | 2000                     |                                 |                                 |                                 | W                               |                                 | 2000                            | 0801 |                          |                          |                          |                          |                          |                   |                   |                   |            |  |
| os      | MAI              | MARPAT 134:178474        |                                 |                                 |                                 |                                 |                                 |                                 |      |                          |                          |                          |                          |                          |                   |                   |                   |            |  |
| GI      |                  |                          |                                 |                                 |                                 |                                 |                                 |                                 |      |                          |                          |                          |                          |                          |                   |                   |                   |            |  |

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AΒ
     RZZ1R1 [I; R = group contg, ≥1 non-H H-bonding atom; R1 = CO2H, or group
     hydrolizable to CO2H; Z = e.g., (hetero)annelated 2-oxo-1-benzazepin-
     1,5-diyl; Z1 = bond, (un)substituted NHCH2, -OCH2, -alkylene, -CH:CH,
     etc.] were prepared Thus, Me 11-methoxycarbonylmethyl-6- oxo-6,11-
     dihydro-5H-dibenz[b,e]azepine-5-acetate (preparation given) was amidated
     by N-(2-aminoethyl)pyridine-2-amine to give, after saponification, title
     compound II. Data for biol. activity of I were given.
IT
     326398-79-2P 326398-84-9P 326398-90-7P
     326399-01-3P 326399-07-9P 326399-11-5P
     326399-17-1P 326399-23-9P 326399-27-3P
     326399-31-9P 326399-36-4P 326399-42-2P
     326399-47-7P, 326399-52-4P 326399-64-8P
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     326399-83-1P 326400-13-9P 326400-18-4P
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     326403-28-5P 326403-32-1P 326403-37-6P
     326403-42-3P 326403-47-8P 326403-51-4P
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     326403-71-8P 326403-76-3P 326404-18-6P
     326404-23-3P 326404-27-7P 326404-31-3P
     326404-36-8P 326471-39-0P
     RL: BAC (Biological activity or effector, except adverse); BSU
(Biological
     study, unclassified); SPN (Synthetic preparation); THU (Therapeutic
use);
     BIOL (Biological study); PREP (Preparation); USES (Uses)
        (preparation of oxobenzazepinealkanoates and analogs as integrin
receptor
        antagonists)
RN
     326398-79-2 CAPLUS
     5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[[2-
CN
(2 -
     pyridinylamino)ethyl]amino]ethyl]- (9CI)
                                                (CA INDEX NAME)
```

сн<sub>2</sub>— со<sub>2</sub>н

RN 326398-84-9 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[4-(2-pyridinyl)-1-piperazinyl]ethyl]- (9CI) (CA INDEX NAME)

RN 326398-90-7 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[6-(1H-benzimidazol-2-yl)-3-pyridinyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo- (9CI) (CA INDEX NAME)

Сн2-со2н

RN 326399-01-3 CAPLUS

yl)amino]ethyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo- (9CI) (CA INDEX NAME)

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Сн2-со2н

RN 326399-07-9 CAPLUS

CN 5H-Dibenz[b,e] azepine-11-acetic acid, 5-[2-[[[6-(4,5-dihydro-1H-imidazol-2-

---- yl)=3=pyridinyl]methyl]amino]=2-oxoethyl]-6,11-dihydro-6-oxo-, monoacetate

(9CI) (CA INDEX NAME)

CM 1

CRN 326399-06-8 CMF C27 H25 N5 O4

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Сн2-со2н

CM 2

CRN 64-19-7 CMF C2 H4 O2

O HO-C-CH3

RN 326399-11-5 CAPLUS

(2-pyridinyl)-4-piperidinyl]methyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 326399-17-1 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[(1H-benzimidazol-2-ylmethyl)amino]-2-oxoethyl]-6,11-dihydro-6-oxo-, monoacetate (9CI) (CA INDEX NAME)

CM 1

CRN 326399-16-0 CMF C26 H22 N4 O4

CM 2

CRN 64-19-7 CMF C2 H4 O2

RN

326399-23-9 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-5-[2-[(1H-imidazo[4.5-

b]pyridin-2-ylmethyl)amino]-2-oxoethyl]-6-oxo-, monoacetate (9CI) (CA INDEX NAME)

CM 1

CRN 326399-22-8 CMF C25 H21 N5 O4

CM 2

CRN 64-19-7

RN 326399-27-3 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[3-oxo-3-[[2-(2-pyridinylamino)ethyl]amino]propyl]- (9CI) (CA INDEX NAME)

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RN 326399-31-9 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[3-oxo-3-[4-(2-pyridinyl)-1-piperazinyl]propyl]- (9CI) (CA INDEX NAME)

CH2-CO2H

RN 326399-36-4 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[3-[[[4-(1H-benzimidazol-2-yl)-2thienyl]methyl]amino]-3-oxopropyl]-6,11-dihydro-6-oxo- (9CI) (CA INDEX NAME)

RN326399-42-2 CAPLUS

CN5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[4-

[(2-

pyridinylamino)methyl]-1-piperidinyl]ethyl]-, monoacetate (9CI) (CA INDEX

NAME)

CM1

CRN 326399-41-1 C29 H30 N4 O4 CMF

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2 CM

CRN 64-19-7 CMF C2 H4 O2

RN 326399-47-7 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[4-[[(phenylmethyl)amino]carbonyl]-1-piperazinyl]ethyl]- (9CI) (CA INDEX NAME)

RN 326399-52-4 CAPLUS

2-

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-{[[5-(1H-benzimidazol-2-yl)-

thienyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo- (9CI) (CA INDEX NAME)

RN 326399-64-8 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[4-(1H-benzimidazol-2-yl)-

2-

thienyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo-, monoacetate (9CI) (CA INDEX NAME)

CM 1

CRN 326399-63-7 CMF C30 H24 N4 O4 S

CM 2

CRN 64-19-7 CMF C2 H4 O2

RN 326399-69-3 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-5-[2-[[[4-(1H-imidazo[4,5-b]pyridin-2-yl)-2-thienyl]methyl]amino]-2-oxoethyl]-6-oxo-(9CI) (CA INDEX NAME)

RN 326399-73-9 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[4-(1H-benzimidazol-2-yl)phenyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo-, monohydrochloride

(9CI) (CA INDEX NAME)

PAGE 1-A

СН2 — СО2Н

HC1

RN 326399-78-4 CAPLUS

CN 25H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[4-(1H-benzimidazol-2-yl)-

thiazolyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo- (9CI) (CA INDEX NAME)

RN 326399-83-1 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[4-(1H-benzimidazol-2-yl)phenyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo- (9CI) (CA INDEX NAME)

RN 326400-13-9 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-5-[2-[[3-(1H-imidazol-2-ylamino)-3-oxopropyl]amino]-2-oxoethyl]-6-oxo- (9CI) (CA INDEX NAME)

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RN 326400-18-4 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[4-[[[[(phenylmethyl)amino]carbonyl]amino]methyl]-1-piperidinyl]ethyl]-(9CI)

(CA INDEX NAME)

RN 326400-23-1 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[3-oxo-3-[[1-

(2-pyridinyl)-4-piperidinyl]methyl]amino]propyl]- (9CI) (CA INDEX NAME)

RN 326400-32-2 CAPLUS

2-

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[3-[[[5-(1H-benzimidazol-2-yl)-

thienyl]methyl]amino]-3-oxopropyl]-6,11-dihydro-6-oxo- (9CI) (CA INDEX NAME)

L Сн2—СО2Н

Сн2—со2н

RN 326400-45-7 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[[4-

CH2-CO2H

RN 326400-50-4 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[4-(2-pyridinylamino)-1-piperidinyl]ethyl]- (9CI) (CA INDEX NAME)

RN 326400-55-9 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[4-(1H-benzimidazol-2-ylamino)phenyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo- (9CI) (CA INDEX NAME)

PAGE 1-A

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RN 326400-60-6 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[4-(1H-benzimidazol-2-ylamino)phenyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo-, methyl ester

(9CI) (CA INDEX NAME)

RN 326400-65-1 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[5-(1H-benzimidazol-2-ylamino)pentyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo- (9CI) (CA INDEX NAME)

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[4-(1H-benzimidazol-2-ylamino)butyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo-(9CI) (CA INDEX NAME)

RN 326400-74-2 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[[3-

[[[(phenylmethyl)amino]carbonyl]amino]phenyl]methyl]amino]ethyl]- (9CI)
(CA INDEX NAME)

RN 326400-79-7 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[4-[(1H-benzimidazol-2-ylamino)methyl]-1-piperidinyl]-2-oxoethyl]-6,11-dihydro-6-oxo-(9CI)

(CA INDEX NAME)

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE RN 326400-88-8 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[[[2-(2-pyridinylamino)-5-thiazolyl]methyl]amino]ethyl]- (9CI) (CA INDEX NAME)

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE RN 326400-94-6 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[2-[(aminoiminomethyl)amino]-4-thiazolyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CRN 326400-93-5 CMF C23 H22 N6 O4 S

CM

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 326400-99-1 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[2[(aminoiminomethyl)amino]5-thiazolyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo- (9CI) (CA
INDEX
NAME)

RN 326401-04-1 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[2-[4-(1H-benzimidazol-2-yl)phenyl]ethyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo- (9CI) (CA INDEX NAME)

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RN 326401-13-2 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-5-[2-[methyl[2-(2-pyridinylamino)ethyl]amino]-2-oxoethyl]-6-oxo- (9CI) (CA INDEX NAME)

CH2-CO2H

CH2-CO2H

RN 326401-32-5 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[4-[(aminoiminomethyl)amino]phenyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-

oxo-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 326401-31-4 CMF C26 H25 N5 O4

СН2-СО2Н

CM2

CRN 76-05-1 CMF C2 H F3 O2

326401-36-9 CAPLUS RN

5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[4-(5-chloro-1H-

benzimidazol-

2-yl)phenyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo- (9CI) INDEX

NAME)

LH2-CO2H

RN 326401-41-6 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[4-(5,6-dimethyl-1H-benzimidazol-2-yl)phenyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo-(9CI) (CA INDEX NAME)

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с<sub>н2-со2н</sub>

RN 326401-46-1 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[[3-(2-pyridinylamino)propyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 326401-54-1 CAPLUS

[2-

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[4-

(2-pyridinylamino)ethyl]-1-piperidinyl]ethyl]- (9CI) (CA INDEX NAME)

RN 326401-59-6 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[3-

[2- (2-pyridinylamino)ethyl]-1-pyrrolidinyl]ethyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 326401-64-3 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[3-[2-

(2-pyridinylamino)ethyl]-1-pyrrolidinyl]ethyl]- (9CI) (CA INDEX NAME)

 $L_{\rm H2-CO2H}$ 

CH2-CO2H

RN 326401-82-5 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[5-[[(phenylmethyl)amino]carbonyl]amino]pentyl]- (9CI) (CA INDEX NAME)

RN 326401-87-0 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[(4-aminophenyl)methoxy]ethyl]-

6,11-dihydro-6-oxo-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)

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RN 326401-92-7 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-[[4[[[(phenylmethyl)amino]carbonyl]amino]phenyl]methoxy]ethyl]- (9CI) (CA
INDEX NAME)

CH2-CO2H

RN 326401-97-2 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[4-[4-[[(phenylmethyl)amino]carbonyl]amino]phenyl]butyl]- (9CI) (CA INDEX NAME)

RN 326402-02-2 CAPLUS

CN 5H-Dibenz[b,e]azepine-5-acetic acid, 11-[2-[[[4-(1H-benzimidazol-2-ylamino)phenyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo-,

## monohydrochloride (9CI) (CA INDEX NAME)

RN 326402-06-6 CAPLUS

1H-

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-5-[2-[[3-(4-methyl-

imidazol-1-yl)propyl]amino]-2-oxoethyl]-6-oxo- (9CI) (CA INDEX NAME)

RN 326402-11-3 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-5-[2-[[3-(4-methyl-1-piperazinyl)propyl]amino]-2-oxoethyl]-6-oxo- (9CI) (CA INDEX NAME)

RN 326402-16-8 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[(3-pyridinylmethyl)amino]ethyl]- (9CI) (CA INDEX NAME)

RN 326402-21-5 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-5-[2-[[3-(1H-imidazol-1-

yl)propyl]amino]-2-oxoethyl]-6-oxo- (9CI) (CA INDEX NAME)

RN 326402-26-0 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-5-[2-[[1-methyl-2-(4-morpholinyl)ethyl]amino]-2-oxoethyl]-6-oxo- (9CI) (CA INDEX NAME)

RN 326402-31-7 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[(1-ethyl-2-pyrrolidinyl)methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo- (9CI) (CA INDEX NAME)

RN 326402-35-1 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[4-

(4 pyridinylmethyl)-1-piperazinyl]ethyl]- (9CI) (CA INDEX NAME)

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Сн2-со2н

CN

[2-

(1-pyrrolidinyl)ethyl]-1-piperazinyl]ethyl]- (9CI) (CA INDEX NAME)

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RN 326402-44-2 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[4-[2-(diethylamino)ethyl]-1-piperazinyl]-2-oxoethyl]-6,11-dihydro-6-oxo- (9CI) (CA INDEX NAME)

RN 326402-48-6 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-5-[2-[4-[2-(4-morpholinyl)ethyl]-1-piperazinyl]-2-oxoethyl]-6-oxo- (9CI) (CA INDEX NAME)

PAGE 1-A

RN 326402-52-2 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[4-(2-

pyrimidinyl)-1-piperazinyl]ethyl]- (9CI) (CA INDEX NAME)

RN 326402-57-7 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[(2-pyridinylmethyl)amino]ethyl]- (9CI) (CA INDEX NAME)

RN 326402-62-4 CAPLUS CN 5H-Dibenz[b,e]azepir

5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-5-[2-[[2-(4-morpholinyl)ethyl]amino]-2-oxoethyl]-6-oxo- (9CI) (CA INDEX NAME)

RN 326402-66-8 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[3-(dibutylamino)propyl]amino]2-oxoethyl]-6,11-dihydro-6-oxo- (9CI) (CA INDEX NAME)

RN 326402-71-5 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[4-(4-pyridinyl)-1-piperazinyl]ethyl]- (9CI) (CA INDEX NAME)

RN 326402-76-0 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-5-[2-[4-[3-(4-morpholinyl)propyl]-1-piperazinyl]-2-oxoethyl]-6-oxo- (9CI) (CA INDEX NAME)

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RN 326402-80-6 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-5-[2-[[3-(2-methyl-1H-

imidazol-1-yl)propyl]amino]-2-oxoethyl]-6-oxo- (9CI) (CA INDEX NAME)

RN 326402-85-1 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[(4-pyridinylmethyl)amino]ethyl]- (9CI) (CA INDEX NAME)

RN 326402-90-8 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-5-[2-[(1-methyl-4-piperidinyl)amino]-2-oxoethyl]-6-oxo- (9CI) (CA INDEX NAME)

RN 326402-94-2 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[[2-(1-piperidinyl)ethyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 326402-99-7 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[4-[3-(1-pyrrolidinyl)propyl]-1-piperazinyl]ethyl]- (9CI) (CA INDEX NAME)

СН2—СО2Н

326403-04-7 CAPLUS RN

1-

CN5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[4-[2-(dimethylamino)ethyl]-

piperazinyl]-2-oxoethyl]-6,11-dihydro-6-oxo- (9CI) (CA INDEX NAME)

326403-08-1 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[4-[3-(dimethylamino)propyl]- 1piperazinyl]-2-oxoethyl]-6,11-dihydro-6-oxo- (9CI) (CA INDEX NAME)

RN 326403-13-8 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[4-[2-(dipropylamino)ethyl]-1piperazinyl]-2-oxoethyl]-6,11-dihydro-6-oxo- (9CI) (CA INDEX NAME)

RN 326403-18-3 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[4-[2-(1-piperidinyl)ethyl]-1-piperazinyl]ethyl]- (9CI) (CA INDEX NAME)

RN 326403-22-9 CAPLUS

CN 15H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[4-[3-(dipropylamino)propyl]-

piperazinyl]-2-oxoethyl]-6,11-dihydro-6-oxo- (9CI) (CA INDEX NAME)

RN 326403-28-5 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[4-(dibutylamino)butyl]amino]2-oxoethyl]-6,11-dihydro-6-oxo- (9CI) (CA INDEX NAME)

RN 326403-32-1 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[4-[2-oxo-2-(1-pyrrolidinyl)ethyl]-1-piperazinyl]ethyl]- (9CI) (CA INDEX NAME)

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RN 326403-37-6 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[3-(diethylamino)propyl]amino]2-oxoethyl]-6,11-dihydro-6-oxo-(9CI) (CA INDEX NAME).

RN 326403-42-3 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[2-(dimethylamino)ethyl]amino]2-oxoethyl]-6,11-dihydro-6-oxo- (9CI) (CA INDEX NAME)

RN 326403-47-8 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[4-(dimethylamino)butyl]amino]2-oxoethyl]-6,11-dihydro-6-oxo- (9CI) (CA INDEX NAME)

RN 326403-51-4 CAPLUS

CN Propanoic acid, 3-[5,6-dihydro-6-oxo-5-[2-oxo-2-[[[4-[[(phenylmethyl)amino]carbonyl]amino]phenyl]methyl]amino]ethyl]-11H-dibenz[b,e]azepin-11-ylidene]-, methyl ester (9CI) (CA INDEX NAME)

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RN 326403-56-9 CAPLUS

CN Propanoic acid, 3-[5,6-dihydro-6-oxo-5-[2-oxo-2-[[[4-[[(phenylmethyl)amino]carbonyl]amino]phenyl]methyl]amino]ethyl]-11H-dibenz[b,e]azepin-11-ylidene]- (9CI) (CA INDEX NAME)

 $^{\rm II}_{\rm CH-CH2-CO2H}$ 

RN326403-61-6 CAPLUS

CN5H-Dibenz[b,e]azepine-11-propanoic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[[[4-[[[(phenylmethyl)amino]carbonyl]amino]phenyl]methyl]amino]ethyl]-, methyl ester (9CI) (CA INDEX NAME)

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LH2-CH2-C-OMe

RN 326403-66-1 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-propanoic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[[4-[[(phenylmethyl)amino]carbonyl]amino]phenyl]methyl]amino]ethyl]-(9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

сн<sub>2</sub>—сн<sub>2</sub>—со<sub>2</sub>н

RN 326403-71-8 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-propanoic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[[2-

(2-pyridinylamino)ethyl]amino]ethyl]-, methyl ester (9CI) (CA INDEX NAME)

LH2-CH2-C-OMe

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Сн2—сн2—со2н

🕨 Na

RN 326404-18-6 CAPLUS

CN 5H-Dibenz[b,e]azepine-ll-acetic acid, 5-[[4-[[[[4-(lH-benzimidazol-2-yl)phenyl]methyl]amino]carbonyl]-2-thiazolyl]methyl]-6,11-dihydro-6-oxo-(9CI) (CA INDEX NAME)

RN 326404-23-3 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[[4-[[4-[(2-pyridinylamino)methyl]-1-piperidinyl]carbonyl]-2-thiazolyl]methyl]
(9CI)

(CA INDEX NAME)

RN 326404-27-7 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[[4-[[[[4-[[[(phenylmethyl)amino]carbonyl]amino]phenyl]methyl]amino]carbonyl]-2-thiazolyl]methyl]- (9CI) (CA INDEX NAME)

326404-31-3 CAPLUS RN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[[4-[[[[4-CN [(2pyridinylamino)methyl]phenyl]methyl]amino]carbonyl]-2-thiazolyl]methyl]-

(9CI) (CA INDEX NAME)

RN 326404-36-8 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[[4-[[[[4-

[(2-

pyridinylamino)methyl]-2-thienyl]methyl]amino]carbonyl]-2thiazolyl]methyl]- (9CI) (CA INDEX NAME)

RN 326471-39-0 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[4-(aminoiminomethyl)-2-thienyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo-, monoacetate (9CI) (CA INDEX NAME)

CM 1

CRN 326471-38-9 CMF C24 H22 N4 O4 S

но\_С\_Сн<sub>3</sub> IT **90664-74-7** 

RL: RCT (Reactant); RACT (Reactant or reagent) (preparation of oxobenzazepinealkanoates and analogs as integrin receptor antagonists)

RN 90664-74-7 CAPLUS

CN Acetic acid, (5,6-dihydro-6-oxo-11H-dibenz[b,e]azepin-11-ylidene)-, methyl ester (9CI) (CA INDEX NAME)

```
IT
    21607-74-9P 90664-75-8P 326404-40-4P
     326404-44-8P 326404-49-3P 326404-53-9P
     326404-66-4P 326404-70-0P 326407-41-4P
     326407-57-2P 326407-61-8P 326407-89-0P
     326407-94-7P 326407-99-2P 326408-04-2P
     326408-08-6P 326408-13-3P 326408-23-5P
     326408-28-0P 326408-33-7P 326408-41-7P
     326408-46-2P 326408-54-2P 326408-59-7P
     326408-63-3P 326408-68-8P 326409-96-5P
     326410-02-0P 326410-07-5P 326410-52-0P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
RACT
     (Reactant or reagent)
        (preparation of oxobenzazepinealkanoates and analogs as integrin
        antagonists)
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RN 21607-74-9 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo- (9CI) (CA INDEX

NAME)

RN 90664-75-8 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-, methyl ester (9CI) (CA INDEX NAME)

RN 326404-40-4 CAPLUS

CN 5H-Dibenz[b,e]azepine-5-acetic acid, 6,11-dihydro-11-(2-methoxy-2-oxoethylidene)-6-oxo-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 326404-44-8 CAPLUS

CN 5H-Dibenz[b,e]azepine-5,11-diacetic acid, 6,11-dihydro-6-oxo-,  $\alpha$ 5-(1,1-dimethylethyl)  $\alpha$ 11-methyl ester (9CI) (CA INDEX NAME)

RN 326404-49-3 CAPLUS

CN 5H-Dibenz[b,e]azepine-5,11-diacetic acid, 6,11-dihydro-6-oxo-,  $\alpha$ 11-methyl ester (9CI) (CA INDEX NAME)

RN 326404-53-9 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 326404-66-4 CAPLUS

CN 5H-Dibenz[b,e]azepine-5-propanoic acid, 11-[2-(1,1-dimethylethoxy)-2-oxoethyl]-6,11-dihydro-6-oxo-, ethyl ester (9CI) (CA INDEX NAME)

RN 326404-70-0 CAPLUS

CN 5H-Dibenz[b,e]azepine-5-propanoic acid, 11-[2-(1,1-dimethylethoxy)-2-oxoethyl]-6,11-dihydro-6-oxo- (9CI) (CA INDEX NAME)

RN 326407-41-4 CAPLUS

CN 5H-Dibenz[b,e]azepine-5,11-diacetic acid, 6,11-dihydro-6-oxo-,  $\alpha$ 11-(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

RN 326407-57-2 CAPLUS

CN 5H-Dibenz[b,e]azepine-5-acetic acid, 6,11-dihydro-11-(3-methoxy-3-oxopropylidene)-6-oxo-(9CI) (CA INDEX NAME)

RN 326407-61-8 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-propanoic acid, 5-(carboxymethyl)-6,11-dihydro-6-

oxo-,  $\alpha$ -methyl ester (9CI) (CA INDEX NAME)

RN 326407-89-0 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[(4-carboxy-2-thiazolyl)methyl]-6,11-dihydro-6-oxo-,  $\alpha$ -(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

326407-94-7 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[[4-(ethoxycarbonyl)-2-

thiazolyl]methyl]-6,11-dihydro-6-oxo-, 1,1-dimethylethyl ester (9CI) (CA

INDEX NAME)

RN

RN 326407-99-2 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[[2-(2-pyridinylamino)ethyl]amino]ethyl]-, methyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN326408-04-2 CAPLUS

CN

CN3-

5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[4-(2-

pyridinyl)-1-piperazinyl]ethyl]-, methyl ester (9CI) (CA INDEX NAME)

326408-08-6 CAPLUS RN

5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[6-(1H-benzimidazol-2-yl)-

pyridinyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo-, methyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

RN 326408-13-3 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[4-[(1,1-dimethylethoxy)carbonyl]-1-piperazinyl]-2-oxoethyl]-6,11-dihydro-6-oxo-, methyl ester (9CI) (CA INDEX NAME)

RN 326408-23-5 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[5-(aminothioxomethyl)-2-thienyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo-, methyl ester

(9CI)

(CA INDEX NAME)

RN 326408-28-0 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[5-(aminoiminomethyl)-2-thienyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo-, methyl ester (9CI)

(CA INDEX NAME)

RN 326408-33-7 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[4-(1H-benzimidazol-2-yl)-2thienyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo-, methyl ester
(9CI)
(CA INDEX NAME)

RN 326408-41-7 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-5-[2-[[3-(1H-imidazol-2-ylamino)-3-oxopropyl]amino]-2-oxoethyl]-6-oxo-, methyl ester (9CI) (CAINDEX NAME)

PAGE 1-A

RN 326408-46-2 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-5-[2-[[[5-[(hydroxyamino)iminomethyl]-2-thienyl]methyl]amino]-2-oxoethyl]-6-oxo-, methyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 326408-54-2 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[5-[[(phenylmethyl)amino]carbonyl]amino]pentyl]-, methyl ester (9CI) (CFINDEX NAME)

RN 326408-59-7 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-5-[2-[(4-nitrophenyl)methoxy]ethyl]-6-oxo-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

IJ

HC1

RN 326408-63-3 CAPLUS

CN

5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-5-[4-(4-nitrophenyl)butyl]-6-oxo- (9CI) (CA INDEX NAME)

RN 326408-68-8 CAPLUS

CN 5H-Dibenz[b,e]azepine-5-acetic acid, 11-[2-[[[4-(1H-benzimidazol-2-ylamino)phenyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 326409-96-5 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-(cyanomethyl)-6,11-dihydro-6-oxo-,

1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 326410-02-0 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-(1-piperazinyl)ethyl]-, methyl ester, mono(trifluoroacetate) (9CI) (CA INDEX

NAME)

CM 1

CRN 326410-01-9 CMF C23 H25 N3 O4

$$CH_2$$
 $CH_2$ 
 $CH_2$ 
 $CH_2$ 
 $CH_2$ 
 $CH_2$ 
 $CH_2$ 
 $CH_2$ 
 $CH_2$ 
 $CH_2$ 

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 326410-07-5 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[4-[(phenylmethyl)amino]carbonyl]-1-piperazinyl]ethyl]-, methyl ester (9CI)

(CA INDEX NAME)

RN 326410-52-0 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-5-(2-hydroxyethyl)-6-oxo-, methyl ester (9CI) (CA INDEX NAME)

L11 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1984:438368 CAPLUS Full-text

DN 101:38368

TI 5,6-Dihydro-11-H-morphanthridin-6-ones and drugs containing them

IN Steiner, Gerd; Friedrich, Ludwig; Lenke, Dieter

PA BASF A.-G., Fed. Rep. Ger.

SO Ger. Offen., 18 pp.

CODEN: GWXXBX

DT Patent

LA German

FAN.CNT 1

| PAN CIVI I           |            |          |                 |          |
|----------------------|------------|----------|-----------------|----------|
| PATENT NO.           | KIND       | DATE     | APPLICATION NO. | DATE     |
| ·                    |            |          |                 |          |
| PI DE 3326641        | <b>A</b> 1 | 19840202 | DE 1983-3326641 | 19830723 |
| PRAI DE 1982-3227934 | Al         | 19820727 |                 |          |
| GI                   |            |          |                 |          |

$$R^2$$
 $CH_2COR^3$ 
 $I$ 

Morphanthridinones I [R1, R2 = H, halo, C1-3 alkyl, CF3; R3 = 1-piperazinyl with N4-(un)substituted by C1-3 alkyl, C2-3 hydroxyalkyl, or F-, C1-, MeO-, or Me-(un)substituted Ph; R3 = C2-4 aminoalkyl, (methyl)morpholinoalkyl] and their physiol. tolerable acid addition salts, useful in treating illnesses accompanied by patholog. increased stomach secretion, e.g., stomach and duodenal ulcers (no data), were prepared Thus, hydrogenating 11-(carbomethoxymethylene)-5,6-dihydromorphanthridin-6-one over 10% Pd/C in MeOH gave 94% 11-(carbomethoxymethyl) analog, which was saponified in refluxing aqueous ethanolic NaOH to give 96% cis,trans-11- (carboxymethyl) analog. This was converted with SOC12 into 99% acid chloride, which reacted with 1-methylpiperazine to give 80% amide II.

IT 90664-74-7

RL: RCT (Reactant); RACT (Reactant or reagent)(hydrogenation of)

RN 90664-74-7 CAPLUS

CN Acetic acid, (5,6-dihydro-6-oxo-11H-dibenz[b,e]azepin-11-ylidene)-, methyl ester (9CI) (CA INDEX NAME)

IT 21607-74-9P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and conversion into acid chloride)

RN 21607-74-9 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo- (9CI) (CA INDEX NAME)

## IT 90664-75-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and saponification of)

RN 90664-75-8 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-, methyl ester (9CI) (CA INDEX NAME)

L11 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1976:180092 CAPLUS Full-text

DN 84:180092

TI Sulfonylureas and sulfonyl semicarbazides with antidiabetic action

IN Winter, Werner; Fauland, Erich; Stach, Kurt; Schmidt, Felix Helmut;
Aumueller, Walter

PA Boehringer Mannheim G.m.b.H., Fed. Rep. Ger.

SO Ger., 8 pp.

CODEN: GWXXAW

DT Patent

LA German

FAN.CNT 1

| r Aun . · | PATENT NO.     | KIND | DATE     | APPLICATION NO. | DATE     |
|-----------|----------------|------|----------|-----------------|----------|
| ΡI        | DE 1618112     | A    | 19720510 | DE 1967-B91627  | 19670315 |
|           | DE 1618112     | B2   | 19750612 | ·               |          |
|           | DE 1618112     | C3   | 19760212 |                 |          |
|           | US 3646009     | Α    | 19720229 | US 1968-711840  | 19680311 |
|           | GB 1153130     | Α    | 19690521 | GB 1968-1153130 | 19680313 |
|           | СН 516535      | Α    | 19711215 | СН 1968-516535  | 19680313 |
|           | СН 516541      | Α    | 19711215 | СН 1968-516541  | 19680313 |
|           | СН 516542      | Α    | 19711215 | СН 1968-516542  | 19680313 |
|           | NL 6803656     | Α    | 19680916 | NL 1968-3656    | 19680314 |
|           | AT 281052      | В    | 19700525 | AT 1968-2545    | 19680314 |
|           | AT 281061      | В    | 19700525 | AT 1969-5843    | 19680314 |
|           | AT 281062      | В    | 19700525 | AT 1969-5844    | 19680314 |
|           | AT 281063      | В    | 19700525 | AT 1969-5845    | 19680314 |
|           | FR 1556173     | Α    | 19690131 | FR 1968-1556173 | 19680315 |
|           | US 3752851 .   | Α    | 19730814 | US 1971-182516  | 19710921 |
| PRAI      | DE 1967-B91627 | Α    | 19670315 |                 | -        |
|           | US 1968-711840 | A3   | 19680311 |                 |          |
| GI        |                |      |          |                 |          |

AB Sulfonylureas I (X=CH2CH2,CH:CH,OCH2, SCH2, O,S, bond; X1=:CH,:CHCH2,:C:CH; R = cycloalkyl, hexamethylenimino, substituted piperidino, tetrahydrothiopyranyl) (34 compds.) were prepared e.g. by treating the carbamates with RNH2. I had 12-16,000 times the antidiabetic activity of 4-H2NC6H4SO2NHCONHBu.

IT 21607-74-9P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 21607-74-9 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo- (9CI) (CA INDEX NAME)

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L11 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2005 ACS on STN
AN
     1969:96656 CAPLUS Full-text
DN
     70:96656
TI
     Oxepin and thiepin derivatives of acetamide
IN
     Winter, Werner; Thiel, Max; Stach, Kurt; Schaumann, Wolfgang;
Ribbentrop,
     Annemarie
     Boehringer, C. F., und Soehne G.m.b.H.
PA
SO
     S. African, 18 pp.
     CODEN: SFXXAB
DT
     Patent
LA
     English
FAN.CNT 1
     PATENT NO.
                         KIND
                                DATE
                                             APPLICATION NO.
                                                                    DATE
     _____
     ZA 6707555
PΙ
                                19680425
     DE 1568217
     FR 1547207
                                             FR
     GB 1144829
                                             GB
PRAI DE
                                19661216
     A mixture of 25.4 q. 6,11-dihydrodibenz[b,e]oxepin-11-ylideneacetic
     acid, m. 114-15°, and 40 ml. SOCl2 was refluxed 2 hrs., evaporated, the
     residue in Et20 mixed with 50 ml. NH3, and the mixture kept overnight
     and worked up to give 79% 11-carboxamidomethylene-6,11-
     dihydrodibenz[b,e]oxepin (I), m. 205° (iso-PrOH). Analogously prepared
     were 82% 5-carboxamidomethyl- 10,11-dihydro-5H-dibenzo[a,d]cycloheptene
     (II), m. 137-8°; 5-carboxamidomethylene-5H-dibenzo[a,d]cycloheptene
     (III), m. 144-5°; 81% 5-carboxamidomethyl analog of III, m. 207-8°; 80%
     theipin analog of I, m. 209-10°; 78% 11-carboxamidomethyl-6,11-dihydrodibenzo[b,e]thiepin, m. 194-5°; 72% 12-carboxamidomethylene-
     7,12-dihydro-6H-dibenzo[b,e]-thiocin, m. 171-3°; 78% 11-
     carboxamidomethylene-2-methyl-6,11-dihydrodibenz[b,e]oxepin, m. 202°;
     11-carboxamidomethyl-2-methyl-6,11-dihydrodibenz[b,e]oxepin, m. 146°;
     and 42% trans - 11 - (1 -carboxamidoethylidene) - 6,11 -
     dihydrodibenz[b,e] - oxepin, m. 188-9° (iso-PrOH-ligroine) (cis isomer
     m. 218-19°, 31%). A solution of 25.3 g. I in 100 ml. tetrahydrofuran
     was treated with 25.3 g. granular Hg-Al, mixed dropwise with 50 ml. H2O,
     and the mixture kept overnight and worked up to give 86% 11-
     carboxamidomethyl-6,11-dihydrodibenz[b,e]oxepin, m. 140-1° (iso-PrOH).
     A mixture of 23.1 g. 5-cyanomethylene-10,11-dihydro-5H-
     dibenzo[a,d]cycloheptene and 23.1 g. KOH in a mixture of 100 ml. each of
     H2O and alc. was refluxed 4 hrs. and worked up to give 85% 5-
     carboxamidomethylene analog of II, m. 166-7^{\circ}. III was prepared in this
     manner also. A solution of 2.7 g. Na in 20 ml. MeOH and 20 ml. HCONMe2
     (DMF) was added to a mixture of 5,6-dihydromorphanthridine-6,11-dione,
     14.6 g. di-Et acetamidophosphonate, and 200 ml. DMF, and the mixture
     stirred 2 hrs. and worked up to give 60% 11-carboxamidomethyl-ene-5,6-
     dihydromorphanthridin-6-one, m. 315-18° (aqueous DMF). Also obtained
     was 5-methyl-11-carboxamidomethylene-5,6-di-hydromorphanthridin-6-one,
     m. 250-2° (EtOH). 5,6-Dihydro-morphanthridin-6-one-11-acetyl chloride
     (IV) (8 g.) in 50 ml. C6H6 was stirred with 200 ml. concentrated aqueous
     NH3 to give 72% corresponding amide, m. 254-5°. A mixture of 11.5 g.
     5,6-dihydro-morphanthridine-6,11-dione and 16.8 g. di-Et
     carbethoxymethyl-phosphonate in 200 ml. DMF was stirred with a solution
     of 2.7 g. Na in 20 ml. MeOH and 20 ml. DMF 2 hrs. and worked up,
     neutralized with HOAc, poured into H2O, and filtered to give 75% 11-
     carbethoxymethylene-5,6-dihydromorphanthridin-6-one, m. 154-5° (iso-
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ProH). A solution of 9 g. of this in 200 ml. MeOH was hydrogenated over Raney Ni at atmospheric pressure to give 77% 11-carbethoxymethyl analog, m. 150-1° (iso-ProH). Saponification of this gave the corresponding acid, m. 267-8° reaction of which with (COCl)2 at ambient temperature gave IV. The subject compds. possess muscle relaxing, tranquilizing, and anticonvulsive activity.

IT 21607-74-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 21607-74-9 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo- (9CI) (CA INDEX

NAME)

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L11 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2005 ACS on STN
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AN 1969:68204 CAPLUS Full-text

DN 70:68204

TI Antidiabetic sulfonylureas and sulfonylsemicarbazides

IN Winter, Werner; Fauland, Erich; Stach, Kurt; Schmidt, Felix Helmut; Aumueller, Walter

PA Boehringer, C. F., und Soehne G.m.b.H.

SO S. African, 28 pp. CODEN: SFXXAB

DT Patent

LA English

FAN.CNT 1

|     | PATENT NO. | KIND | DATE     | APPLICATION NO. | DATE |
|-----|------------|------|----------|-----------------|------|
|     |            |      |          |                 |      |
| PΙ  | ZA 6801636 |      | 19680812 |                 |      |
|     | DE 1618112 |      |          | DE              |      |
|     | FR 1556173 |      |          | FR              |      |
|     | GB 1153130 |      |          | GB              |      |
|     | US 3646009 |      | 19720000 | US              |      |
|     | US 3752851 |      | 19730000 | US              |      |
| PRA | I DE       |      | 19670315 |                 |      |
|     |            |      |          |                 |      |

AB A solution of 4.5 g. p-[2-[2-(fluoren-9-

yl)acetylamino]ethyl]phenylsulfonylca rbamic acid Et ester, 100 ml. anhydrous PhMe, and 10 ml. HCONMe2 was added to 1.3 g. 4methylcyclohexylamine at 80°, the mixture boiled 15 min., cooled, and shaken with 300 ml. 0.2N NaOH, the precipitate suction-filtered off, washed with ether, and dissolved in 1:1 acetone-H2O, the solution diluted with H2O and acidified to pH 5.5 by addition of dilute HCl to give 74% I (Y = bond line, X = CHCH2, R = 4-methylcyclohexyl (Q)], m. 198-9° (MeOH). Similarly prepared I were (Y, X, R, % yield, and m.p. given): bond line, CHCH2, 4,4-dimethylpiperidino (Z), 58, 163-4°; bond line, CHCH2, 4-methylpiperidino (A), 76, 132-3°; CH2O, C:CH, Z, 53, 183-4°; CH2O, C:CH, Q, 65, 216-17°; CH2O, CHCH2, Q, 65, 216-17°; CH2O, CHCH2, Z, 44, 202-3°; O, CHCH2, Q, 48, 208-10°; O CHCH2, A, 45, 128-30°; CH2O, C:CMe, Q, 42, - (K salt m.  $161-3^{\circ}$ ); S, CHCH2, Z, 55, - [K salt m. 172-4° (decomposition)]; bond line, CHCH2, bicyclo[2.2.1]hept-2-yl, 58, 191-3°; bond line, CHCH2, cyclooctyl, 52, 192-3°; bond line, CHCH2, 1adamantyl, 64, 201-2°; bond line, CHCH2, 1-cycloheptyl, 49, 178-80°. A mixture of 4 g. p-[2-(2-(6,11-dihydrodibenz[b,e]-oxepin-11y1)acetylamino)ethyl]benzenesulfonamide and 2.5 g. ground K2CO3 in 100 ml. acetone was boiled and stirred 30 min., 1.5 g. cyclohexyl isocyanate added dropwise, the mixture refluxed and stirred 2 hrs., solvent distilled, residue taken up in H2O, clarified with charcoal, and filtered, and the filtrate acidified with dilute HCl to precipitate 66% I [Y = CH2O, X = CHCH2, R = cyclohexyl (E)], m.  $201-2^{\circ}$  (alc.). ylidene) - acetylamino]ethyl]benzenesulfonamide, m. 215-16°. 3-[p-(2-Aminoethyl)phenylsulfonyl]-1-cyclohexylurea (6.5 g.; m. 211-12°) was suspended in 75 ml. pyridine and mixed with 5 g. xanthene-9-carboxylic acid chloride, the mixture kept 48 hrs., solvent distilled in vacuo, residue digested in dilute HCl, the solid filtered off by suction, washed with water, and purified by dissoln. in 0.2N NaOH and repptn. with dilute HCl to give 81% I (Y = O, X = CH, R = E),  $m.~218-20^{\circ}$  (MeOH). Similarly prepared were: I (Y = CH2CH2, X = CH, R = E), m.  $202-3^{\circ}$ , and I (Y = CH2S, X = CHCH2, R = A), m. 222-3°, from p-(H2NCH2CH2)C6H4SO2NHCONHA, m. 210-12°, and 6,11-

dihydrodibenzo[b,e]thiepin-11-ylacetyl chloride. A mixture of 4.5 q. p-[2-(2-(thiaxanthen - 9 -yl)acetylamino)ethyl]benzenesulfonamide and an equimolar amount NaH in 20 ml. HCONMe2 was stirred 10 min., 2.0 g. pyrocarbonic acid diethyl ester added, the mixture kept 10-15 min., and 0.36 g. HCl in absolute EtOH added to give a solution of p-[2-(2thiaxanthen-9- yl)acetylamino)ethyl]-phenylsulfonylcarbamic acid Et ester. To this solution was added 1.4 q. 4-methylcyclohexylamine in 100 ml. PhMe, the mixture boiled 25 min., cooled, and shaken with 0.2N NaOH, and dilute HCl added to precipitate 55% I (Y = S, X = CHCH2, R = O), m. 198-9° (MeOH). Similarly prepared were I (Y, X, R, % yield, and m.p. given): S, CHCH2, Z, 48, 175-6°; bond line, C:CH, A, 63, 155-6°; CH2S, C:CH, Q, 70, 189-90°; CH2S, C:CH, A, 74, 210-11°; bond line, C:CH, Q, 72, 210-12°; CH:CH, CHCH2, Q, 67, 174-5°; bond line, NCH2, E, 64, 196-8°; bond line, NCH2, Q, 73, 198-200°; bond line, NCH2, A, 58, 154-6°; bond line, NCH2CH2, Q, 63, 206-8°; CH2CH2, C:CH, Q, 51, 194-5°; CH2CH2, CHCH2, Q, 63, 204-6°; CH2S, CHCH2, Q, 51, 153-5°; CH2S, CHCH2, Z, 50, 226-8°; CH2O, CHCH2, A, 48, 198-200°; bond line, CH, A, 62, 172-3°; bond line, CHCH2CH2, E, 60, 207-8°; bond line, CHCH2CH2, Q, 59, 210-12; bond line, CHCH2CH2, Z, 52, 156-8°. Similarly prepared II were (Y, X, R, R1, R1, % yield, and m.p. given): CH2O, CHCH2, Q, MeO, H, 67, 172-4 CHCH2, Q, Me, H, 56, 179-80°; CH2O, CHCH2, Q, Cl, H, 72, 210-12°; bond line, CHCH2, Q, H, Me, 75, 202-3°; bond line, CHCH2, Q, H, MeO, 58, 168-9°; bond line, CHCH2, Q, H, Cl, 69, 218-20°. Similarly prepared was 71% 1-(4-methylcyclohexyl)-3-[p-(2-(2-(6,7-dihydro-12H-dibenzo[b,e]thiocin - 12 - yl)acetylamino)ethyl)- phenylsulfonyl]urea, m. 184-6°. Similarly prepared I from the Na salt of p-[2-(2-(fluoren-9yl)acetylamino)ethyl]benzenesulfonamide were (Y, X, R, % yield, and m.p. given): bond line, CHCH2, 4-methoxycyclohexyl, 61%, 196-7°; bond line, CHCH2, tetrahydrothiapyran-4-yl, 53, 221-2°; bond line, CHCH2, 4,4dimethylcyclohexyl, 67, 197-8°; bond line, CHCH2, 2-phenylethyl, 55, 186-7°; bond line, CHCH2, E, 54, 205-5°. Similarly prepared was 72% 1,1-hexamethylene-4-[p-(2-(2-(fluoren-9-yl)acetylamino)ethyl)phenylsulfon yl]semicarbazide, m. 110-12°. To prepare the acylaminoethylbenzenesulfonamides, 1 mole of the carboxylic acid chloride in question, dissolved in CH2Cl2, was added dropwise with stirring to a solution of 1 mole p-(H2NCH2CH2)-C6H4SO2NH2, and 2 moles Na2CO3 in H2O, the mixture stirred 1-2 hrs., dilute NaOH and H2O added to pH 10-11, CH2C12 separated, and dilute HCl added to pH 8.8 to precipitate product which can be recrystd. from dilute alc. or 10:1:6 alc.-HCONMe2-H2O. To prepare the acylaminoethylphenylcarbamic acid Et esters, 1 mole of the acylaminoethylbenzenesulfonamide was dissolved in HCONMe2, mixed with 1 mole NaH, cooled, stirred 20 min., 1.2 mole pyrocarbonic acid diethyl ester added, the mixture heated and stirred at 60°, after cessation of CO2 evolution, the solvent vacuum distilled, the residue dissolved in H2O, and dilute HCl added to pH 2-4 to precipitate product which may be recrystd. from alc. III and IV prepared were [Y, X, m.p. III, m.p. IV (R = H), and m.p. IV (R = CO2Et) given]: bond line, C:CH, 229-31°, 215-16°, -; bond line, CHCH2, 139-41°, 207-9°, 135-6°; 0, CHCH2, 158-9°, 236-8°, 162-4°; S, CHCH2, 170-1°, 208-9°, 137-9°; CH20, C:CH,  $185-6^{\circ}$ ,  $238-9^{\circ}$ ,  $196-7^{\circ}$ ; CH2O, CHCH2,  $117-19^{\circ}$ ;  $178-9^{\circ}$ , -; CH2O, C:CMe, 178°, -, 128-30°; CH2S, C:CH, 179-81°, 210-12°, -; CH2S, CHCH2, 208-9°, 167-9°, -; CH:-CH, CHCH2, 167-8°, 197-8°, -; CH2CH2, CHCH2, 162-4°, 194-5°, -; CH2CH2, C:CH, 167-8°, 197-8°, -; bond line, NCH2, 215°, 254-5°, -; bond line, NCH2CH2, 166-8°, 173°, -; bond line, CH, 218-20°, 234-6°, -; bond line, CHCH2CH2, 145-6°, 186-8°, -. V and VI prepared were (Y, X, R1, R2, m.p. V, and m.p. VI given): bond line, CHCH2, H, Me, 126-7°, 210-11°; bond line, CHCH2, H, MeO, 170-1°, 158-60°; bond line,

CHCH2, C1, H, -, 212-13°; CH2O, CHCH2, MeO, H, 119-20°, 138-40°; CH2O, CHCH2, Me, H, 110-11°, 169-70°; CH2O, CHCH2, C1, H, 211-12°, 190-2°. Similarly prepared were: 6.7-dihydro-12H-dibenzo[b,e]thiocin- 12-ylacetic acid, m. 193°, p-[2-(2-(6.7-dihydro-12H-dibenzo[b,e]thiocin-12-yl)acetylamino) ethyl]benzenesulfonamide, m. 163-5°, 6.7-dihydro-12H-dibenzo-[b,e]thiocin-12-ylideneacetic acid, m. 200-2°, and 6-oxo-5.6-dihydro-11H-dibenz[b,e]azepin-11-ylacetic acid, m. 267-8°.

IT 21607-74-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

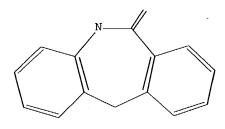
RN 21607-74-9 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo- (9CI) (CA INDEX

NAME)

L3

(FILE 'HOME' ENTERED AT 16:21:12 ON 06 JAN 2005) FILE 'CAPLUS' ENTERED AT 16:21:19 ON 06 JAN 2005 L11 S WO2001010847/PN L2 SEL L1 1- RN : 284 TERMS FILE 'STNGUIDE' ENTERED AT 16:21:46 ON 06 JAN 2005 FILE 'REGISTRY' ENTERED AT 16:22:44 ON 06 JAN 2005 L3STRUCTURE UPLOADED 284 S L2 T.4 Ľ5 7 S L3 SUB=L4 SAM 133 S L3 FUL SUB=L4 L6 FILE 'CAPLUS' ENTERED AT 16:23:48 ON 06 JAN 2005 T.7 61 S L6 FILE 'STNGUIDE' ENTERED AT 16:24:01 ON 06 JAN 2005 FILE 'REGISTRY' ENTERED AT 16:25:03 ON 06 JAN 2005  $^{\mathrm{F8}}$ STRUCTURE UPLOADED L9 6 S L8 SAM SUB=L6 L10132 S L8 FUL SUB=L6 FILE 'CAPLUS' ENTERED AT 16:26:06 ON 06 JAN 2005 L11 6 S L10 => d 13; d 18; log y L3 HAS NO ANSWERS



STR

Structure attributes must be viewed using STN Express query preparation.

L8 HAS NO ANSWERS
L8 STR

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

Structure attributes must be viewed using STN Express query preparation.

SINCE FILE COST IN U.S. DOLLARS TOTAL ENTRY SESSION FULL ESTIMATED COST 31.44 247.69 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION CA SUBSCRIBER PRICE -4.38-4.38

STN INTERNATIONAL LOGOFF AT 16:28:24 ON 06 JAN 2005

elected gung

- L7 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2005 ACS on STN
- AN 2002:142712 CAPLUS Full-text
- DN 136:200186
- TI Preparation of dibenzo[b,e]azepines as  $\alpha V\beta 3$  integrin ligands
- IN Geneste, Herve; Kling, Andreas; Lauterbach, Arnulf; Graef, Claudia Isabella; Subkowski, Thomas; Hornberger, Wilfried
- PA Basf Aktiengesellschaft, Germany
- SO PCT Int. Appl., 157 pp. CODEN: PIXXD2
- DT Patent
- LA German
- FAN.CNT 9

| FAN.CNT 9 |                   |                  |      |             |             |                |                |                 |                |            |      |               |          |          |          |          |     |     |
|-----------|-------------------|------------------|------|-------------|-------------|----------------|----------------|-----------------|----------------|------------|------|---------------|----------|----------|----------|----------|-----|-----|
|           | PATENT NO.        |                  |      | KIND        |             | DATE           |                | APPLICATION NO. |                |            |      |               |          | DATE     |          |          |     |     |
| PI        |                   |                  |      |             |             | WO 2001-EP9224 |                |                 |                |            |      | 20010809      |          |          |          |          |     |     |
|           | WO                | 2002014320       |      |             |             |                |                |                 |                |            |      |               |          |          |          |          |     |     |
|           |                   | W:               | ΑE,  | AG,         | AL,         | AM,            | ΑT,            | AU,             | ΑZ,            | BA,        | BB,  | BG,           | BR,      | BY,      | ΒZ,      | CA,      | CH, | CN, |
|           |                   |                  | co,  | CR,         | CU,         | CZ,            | DE,            | DK,             | DM,            | DZ,        | EC,  | EE,           | ES,      | FΙ,      | GB,      | GD,      | GE, | GH, |
|           |                   |                  | GM,  | HR,         | HU,         | ID,            | IL,            | IN,             | IS,            | JP,        | KE,  | KG,           | KΡ,      | KR,      | ΚZ,      | LC,      | LK, | LR, |
|           |                   |                  | LS,  | LT,         | LU,         | LV,            | MA,            | MD,             | MG,            | MK,        | MN,  | MW,           | MX,      | MZ,      | NO,      | NΖ,      | PL, | PT, |
|           |                   |                  | RO,  | RU,         | SD,         | SE,            | SG,            | SI,             | SK,            | SL,        | ТJ,  | TM,           | TR,      | TT,      | TZ,      | UA,      | UG, | US, |
|           |                   |                  | UZ,  | VN,         | YU,         | ZA,            | ZW,            | AM,             | ΑZ,            | BY,        | KG,  | KΖ,           | MD,      | RU,      | ТJ,      | TM       |     |     |
|           |                   | RW:              | GH,  | GM,         | KE,         | LS,            | MW,            | ΜZ,             | SD,            | SL,        | SZ,  | TZ,           | UG,      | ZW,      | AT,      | BE,      | CH, | CY, |
|           |                   |                  | DE,  | DK,         | ES,         | FI,            | FR,            | GB,             | GR,            | IE,        | IT,  | LU,           | MC,      | NL,      | PT,      | SE,      | TR, | BF, |
|           |                   |                  | ВJ,  | CF,         | CG,         | CI,            | CM,            | GA,             | GN,            | GQ,        | GW,  | ML,           | MR,      | NE,      | SN,      | TD,      | TG  |     |
|           | DE                | 1003             | 9998 |             |             | A1             |                | 2002            | 0221           |            | DE 2 | 2000-10039998 |          |          |          | 20000811 |     |     |
|           | AU                | J 2001091756     |      |             | A5 20020225 |                |                | AU 2001-91756   |                |            |      |               |          | 20010809 |          |          |     |     |
|           | CA                |                  |      |             |             |                |                | CA 2001-2419078 |                |            |      |               |          | 20010809 |          |          |     |     |
|           | EP                | 2 1307443        |      |             | A2          | A2 20030507    |                |                 | EP 2001-971899 |            |      |               |          |          | 20010809 |          |     |     |
|           |                   | R:               | AT,  | BE,         | CH,         | DE,            | DK,            | ES,             | FR,            | GB,        | GR,  | IT,           | LI,      | LU,      | NL,      | SE,      | MC, | PT, |
|           |                   |                  | ΙE,  | SI,         | LT,         | LV,            | FI,            | RO,             | MK,            | CY, AL, TR |      |               |          |          |          |          |     |     |
|           | JP                | 2004506637       |      |             | T2 20040304 |                |                | JP 2002-519460  |                |            |      |               |          | 20010809 |          |          |     |     |
|           | US 2004077638     |                  |      | A1 20040422 |             |                | US 2003-344449 |                 |                |            |      |               | 20030908 |          |          |          |     |     |
| PRAI      | DE                | DE 2000-10039998 |      |             | 8           | A 20000811     |                |                 |                |            |      |               |          |          |          |          |     |     |
|           | DE 2000-10028575  |                  |      | 5           | A.          | A 20000614     |                |                 |                |            |      |               |          |          |          |          |     |     |
|           | WO 2001-EP9224 W  |                  |      |             |             |                | 2001           | 0809            |                |            |      |               |          |          |          |          |     |     |
| os        | MARPAT 136:200186 |                  |      |             |             |                |                |                 |                |            |      |               |          |          |          |          |     |     |
| GI        |                   |                  |      |             |             |                |                |                 |                |            |      |               |          |          |          |          |     |     |

$$Q^{1} = -Ar \underbrace{ \begin{bmatrix} W \\ X \end{bmatrix}}_{i|} D$$

The invention relates to novel compds. which bind to integrin receptors, in particular as ligands for the  $\alpha V\beta 3$  integrin receptor, the use thereof and pharmaceutical prepns. containing said compds. BGL [L = UT; T = CO2H, group hyrdolyzable to CO2H, isostere of CO2H; U = Xa(CR1R2)b, CR1:CR2, C.tplbond.C, etc.; a = 0, 1; b = 0-2; X = CR3R4, NR5, O, S; R1-R4 = T, H, OH, CONH2, halo, amino, substituted alkyl, alkenyl, alkynyl, cycloalkyl, alkylaminocarbonyl, etc.; R5 = H, (substituted) alkyl,

cycloalkyl, alkoxycarbonyl, alkylsulfonyl, etc.; G = Q1; Ar = atoms to form a (substituted) (anellated) (heterocyclylic) 3-10 membered aryl ring; D = atoms to form a (substituted) (anellated) (unsatd.) (aromatic) 3-10 membered (heterocyclyl) ring; X = CR11, N, C; W = YNR15; Y = CO, CS, C:NR12, CR13R14; R11 = H, halo, OH, (substituted) alkyl, alkoxy; R12 = H, OH, (substituted) alkyl, alkoxy, cycloalkyl, cycloalkoxy, aryl, aryloxy, aralkyl, aralkoxy; R13, R14 = H, (substituted) alkyl, alkenyl, alkynyl, alkoxy; R13R14 = OCH2CH2O, OCH2O, (substituted) cycloalkyl; R15 = R151, AR152, etc.; R151 = COR152, CSR152, NO2, tetrazolyl, etc.; R152 = H, (substituted) cycloalkyl, aryl, heteroaryl, etc.; R153 = H, OH, (substituted) alkyl, alkoxy, aralkyl, aralkoxy, etc.; B = structure element containing ≥1 atom which can function as an acceptor in H bond formation under physiol. conditions], were prepared as  $\alpha V\beta 3$  integrin ligands (no data). Thus, ethyldiisopropylamine and HATU were added to a 0° solution of 11-(2-methoxy-2-oxoethyl)-5-methyl-6-oxo- 6,11-dihydro-5H-dibenzo[b,e]azepine-3-carboxylic acid (preparation given) in CH2Cl2; the mixture was stirred 1 h at  $0^{\circ}$  and 7-(4-aminobutyl)-1,2,3,4tetrahydro[1,8]naphthyridine bistrifluoroacetate and ethyldiisopropylamine were added followed by stirring for 1 h at 0° overnight at room temperature to give Me [5-methyl-6-oxo-3-[[4-[5,6,7,8- tetrahydro[1,8]naphthyridin-2-yl]butyl]amino]carbonyl]-6,11dihydro-5H- dibenzo[b,e]azepin-11-yl]acetate.

400712-67-6P 400712-68-7P 400712-69-8P 400712-70-1P 400712-71-2P 400712-72-3P 400712-73-4P 400712-74-5P 400712-75-6P 400712-78-9P 400712-79-0P 400712-82-5P 400712-83-6P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of dibenzoazepines as  $\alpha V\beta 3$  integrin ligands) 400712-67-6 CAPLUS 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-5-methyl-6-oxo-3-[4-

pyridinylamino)butoxy] - (9CI) (CA INDEX NAME)

RN

CN (2-

RN

CN (2400712-68-7 CAPLUS
5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-5-methyl-6-oxo-3-[3-pyridinylamino)propoxy]-, monosodium salt (9CI) (CA INDEX NAME)

Na

RN 400712-69-8 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 3-[[[[4-(1H-benzimidazol-2-ylamino)phenyl]methyl]amino]carbonyl]-6,11-dihydro-5-methyl-6-oxo-, monosodium salt (9CI) (CA INDEX NAME)

Na

RN 400712-70-1 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-5-methyl-6-oxo-3-[[[3-

(2-pyridinylamino)propyl]amino]carbonyl]-, monosodium salt (9CI) (CA INDEX NAME)

Na

N 400712-71-2 CAPLUS

CN Acetic acid, [3-[[[[4-(1H-benzimidazol-2-ylamino)phenyl]methyl]amino]carbo

nyl]-5,6-dihydro-5-methyl-6-oxo-11H-dibenz[b,e]azepin-11-ylidene]-, methyl

ester (9CI) (CA INDEX NAME)

RN 400712-72-3 CAPLUS

Acetic acid, [3-[[[[4-(1H-benzimidazol-2-

ylamino)phenyl]methyl]amino]carbo

nyl]-5,6-dihydro-5-methyl-6-oxo-11H-dibenz[b,e]azepin-11-ylidene]- (9CI) (CA INDEX NAME)

400712-73-4 CAPLUS

Acetic acid, [5,6-dihydro-5-methyl-6-oxo-3-[3-(2-

pyridinylamino)propoxy]-

11H-dibenz[b,e]azepin-11-ylidene]-, monosodium salt (9CI) (CA INDEX NAME)

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 3-[[[5-(1H-benzimidazol-2-ylamino)pentyl]amino]carbonyl]-6,11-dihydro-5-methyl-6-oxo-, monosodium salt (9CI) (CA INDEX NAME)

Na

RN 400712-75-6 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 3-[[(1H-benzimidazol-2-ylmethyl)amino]carbonyl]-6,11-dihydro-5-methyl-6-oxo-, monosodium salt (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
 & \text{Me} \\
\hline
 & \text{C} \\
\hline
 & \text{NH-CH}_2
\end{array}$$

Na

RN 400712-78-9 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 3-[[[[trans-4-(1H-benzimidazol-2-ylamino)cyclohexyl]methyl]amino]carbonyl]-6,11-dihydro-5-methyl-6-oxo-, methyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 400712-79-0 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 3-[[[[trans-4-(1H-benzimidazol-2-ylamino)cyclohexyl]methyl]amino]carbonyl]-6,11-dihydro-5-methyl-6-oxo-(9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 400712-82-5 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 3-[[[4-(1H-benzimidazol-2-ylamino)butyl]amino]carbonyl]-6,11-dihydro-5-methyl-6-oxo-, methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
 & \text{Me} \\
 & \text{NH} \quad \text{(CH}_2)} & \text{4-NH} \quad \text{MN} \\
 & \text{CH}_2 - \text{C-OMe} \\
 & \text{O} \\
 & \text{NH} \quad \text{(CH}_2)} & \text{4-NH} \\
 & \text{NH} \quad \text{(CH}_2)} & \text{3-NH} \\
 & \text{(CH}_2)$$

RN 400712-83-6 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 3-[[[4-(1H-benzimidazol-2-ylamino)butyl]amino]carbonyl]-6,11-dihydro-5-methyl-6-oxo- (9CI) (CA INDEX NAME)

IT 400712-92-7P 400712-93-8P 400712-94-9P 400712-95-0P 400712-96-1P 400712-99-4P

## 400713-00-0P 400713-04-4P 400713-05-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

(preparation of dibenzoazepines as  $\alpha V\beta 3$  integrin ligands)

RN 400712-92-7 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-5-methyl-3-[4-[(1-oxido-

2-pyridinyl)amino]butoxy]-6-oxo-, methyl ester (9CI) (CA INDEX NAME)

RN 400712-93-8 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-5-methyl-6-oxo-3-[4-

(2-

pyridinylamino)butoxy]-, methyl ester (9CI) (CA INDEX NAME)

RN 400712-94-9 CAPLUS

CN Acetic acid, [5,6-dihydro-5-methyl-3-[3-[(1-oxido-2-

pyridinyl)amino]propoxy]-6-oxo-11H-dibenz[b,e]azepin-11-ylidene]-,
methyl

ester (9CI) (CA INDEX NAME)

RN 400712-96-1 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-5-methyl-6-oxo-3-[3-(2-pyridinylamino)propoxy]-, methyl ester (9CI) (CA INDEX NAME)

RN 400712-99-4 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 3-[[[[4-(1H-benzimidazol-2-ylamino)phenyl]methyl]amino]carbonyl]-6,11-dihydro-5-methyl-6-oxo-, methyl
ester (9CI) (CA INDEX NAME)

RN 400713-00-0 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-5-methyl-6-oxo-3-[[[3-

(2-pyridinylamino)propyl]amino]carbonyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 400713-04-4 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 3-[[[5-(1H-benzimidazol-2-ylamino)pentyl]amino]carbonyl]-6,11-dihydro-5-methyl-6-oxo-, methyl ester

(9CI) (CA INDEX NAME)

RN 400713-05-5 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 3-[[(1H-benzimidazol-2-ylmethyl)amino]carbonyl]-6,11-dihydro-5-methyl-6-oxo-, methyl ester (9CI)

(CA INDEX NAME)

L7 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2002:97692 CAPLUS Full-text

DN 137:103383

TI Synthesis and SAR of N-substituted dibenzazepinone derivatives as novel potent and selective  $\alpha V\beta 3$  antagonists

AU Kling, Andreas; Backfisch, Gisela; Delzer, Jurgen; Geneste, Herve; Graef, Claudia; Holzenkamp, Uta; Hornberger, Wilfried; Lange, Udo E. W.; Lauterbach, Arnulf; Mack, Helmut; Seitz, Werner; Subkowski, Thomas

CS Knoll GmbH, Ludwigshafen, D-67008, Germany

SO Bioorganic & Medicinal Chemistry Letters (2002), 12(3), 441-446 CODEN: BMCLE8; ISSN: 0960-894X

PB Elsevier Science Ltd.

DT Journal

LA English

OS CASREACT 137:103383

GΙ

AB Substituted oxodibenzazepineacetic acids substituted with guanidines or guanidine pharmacophores such as I are prepared as potential  $\alpha V\beta 3$  (vitronectin receptor) antagonists. The oxodibenzazepineacetic acid core II is prepared in 5 steps from 9,10-anthraquinone; coupling of II with guanidine or guanidine pharmacophore-substituted amines such as III followed by hydrolysis of the Me ester yields compds. such as I. Structure-activity relationships are determined for the guanidine or guanidine pharmacophore-substituted oxodibenzazepineacetic acids, varying the linker between the guanidine pharmacophore and the oxodibenzazepine and the choice of guanidine pharmacophore. Compound I and a second guanidine pharmacophore-substituted oxodibenzazepineacetic acid are found to be highly active inhibitors of the vitronectin receptor in vitro and are found to be bioavailable in ADME assays.

IT 326401-69-8P 326401-92-7P 443332-42-1P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation of a guanidine or guanidine pharmacophore-substituted

oxodibenzazepineacetic acid and lack of activity as a potential  $\alpha V\beta 3$  receptor antagonist)

RN 326401-69-8 CAPLUS

CN 5H-Dibenz[b,e] azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[[4-

NAME)

PAGE 1-A

PAGE 2-A

L Сн2-со2н

RN 326401-92-7 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-[[4-[[(phenylmethyl)amino]carbonyl]amino]phenyl]methoxy]ethyl]- (9CI) (CP INDEX NAME)

Сн2-со2н

RN 443332-42-1 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-[[[4-[[(phenylmethyl)amino]carbonyl]amino]phenyl]methyl]amino]ethyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

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ΙT
     326398-90-7P 326399-16-0P 326399-52-4P
     326399-63-7P 326399-69-3P 326399-78-4P
     326399-83-1P 326400-55-9P 326400-65-1P
     326400-70-8P 326401-04-1P 326401-08-5P
     326401-18-7P 326401-26-7P 326401-31-4P
     326401-36-9P 326401-41-6P 326401-74-5P
     326401-97-2P 326471-38-9P 443332-00-1P
     443332-07-8P 443332-29-4P 443332-52-3P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL
     (Biological study); PREP (Preparation)
        (preparation of guanidine or guanidine pharmacophore-substituted
        oxodibenzazepineacetic acids as potential \alpha V\beta 3 receptor
        antagonists)
     326398-90-7 CAPLUS
RN
     5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[6-(1H-benzimidazol-2-y1)-
CN
3-
     pyridinyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo- (9CI) (CA INDEX
     NAME)
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PAGE 1-A

CH2-CO2H

RN 326399-16-0 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[(1H-benzimidazol-2-ylmethyl)amino]-2-oxoethyl]-6,11-dihydro-6-oxo- (9CI) (CA INDEX NAME)

RN 326399-52-4 CAPLUS

2-

2-

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[5-(1H-benzimidazol-2-yl)-

thienyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo- (9CI) (CA INDEX NAME)

RN 326399-63-7 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[4-(1H-benzimidazol-2-yl)-

thienyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo- (9CI) (CA INDEX

RN 326399-69-3 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-5-[2-[[[4-(1H-imidazo[4,5-b]pyridin-2-yl)-2-thienyl]methyl]amino]-2-oxoethyl]-6-oxo-(9CI) (CA INDEX NAME)

RN 326399-78-4 CAPLUS

2-

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[4-(1H-benzimidazol-2-yl)-

thiazolyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo- (9CI) (CA INDEX NAME)

RN 326399-83-1 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[4-(1H-benzimidazol-2-yl)phenyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo- (9CI) (CA INDEX NAME)

RN 326400-55-9 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[4-(1H-benzimidazol-2-ylamino)phenyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo-(9CI) (CA INDEX NAME)

RN 326400-65-1 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[5-(1H-benzimidazol-2-ylamino)pentyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo- (9CI) (CA INDEX NAME)

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[4-(1H-benzimidazol-2-

ylamino)butyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo- (9CI) (CA INDEX NAME)

RN 326401-04-1 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[2-[4-(1H-benzimidazol-2-yl)phenyl]ethyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo- (9CI) (CA INDEX NAME)

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PAGE 2-A

PAGE 1-A

PAGE 2-A

RN 326401-18-7 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2[[[4(2-pyridinylamino)phenyl]methyl]amino]ethyl]- (9CI) (CA INDEX NAME)

 $L_{\rm H2-CO2H}$ 

RN 326401-31-4 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[4[(aminoiminomethyl)amino]phenyl]methyl]amino]-2-oxoethyl]-6,11-dihydro6oxo- (9CI) (CA INDEX NAME)

CH2-CO2H

RN 326401-36-9 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[4-(5-chloro-1H-benzimidazol2-yl)phenyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo- (9CI) (CA INDEX
NAME)

CH2-CO2H

RN 326401-41-6 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[4-(5,6-dimethyl-1H-benzimidazol-2-yl)phenyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo-(9CI) (CA INDEX NAME)

PAGE 1-A

L Сн2-со2н

RN 326401-74-5 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[[[4-

[[(phenylmethoxy)carbonyl]amino]phenyl]methyl]amino]ethyl]- (9CI) (CA INDEX NAME)

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Сн2-со2н

RN 326401-97-2 CAPLUS

CN

5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[4-[4-[[([(phenylmethyl)amino]carbonyl]amino]phenyl]butyl]- (9CI) (CA INDEX NAME)

RN 326471-38-9 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[4-(aminoiminomethyl)-2-thienyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo- (9CI) (CA INDEX NAME)

RN 443332-00-1 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[4-(1H-benzimidazol-2-yl)phenyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo- (9CI) (CA INDEX NAME)

L Сн<sub>2</sub>—со<sub>2</sub>н

RN 443332-07-8 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[3-(1H-benzimidazol-2-yl)phenyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo- (9CI) (CA INDEX NAME)

RN

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L СН2— СО2Н

RN 443332-52-3 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[trans-4-(1H-benzimidazol-2ylamino)cyclohexyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo- (9CI)
(CA INDEX NAME)

Relative stereochemistry.

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IT
     326400-60-6P 326401-22-3P 326408-08-6P
     326408-33-7P 443331-29-1P 443331-31-5P
     443331-34-8P 443331-37-1P 443331-42-8P
     443331-47-3P 443331-50-8P 443331-53-1P
     443331-56-4P 443331-59-7P 443331-62-2P
     443331-65-5P 443331-68-8P 443331-73-5P
     443331-76-8P 443331-79-1P 443331-84-8P
     443331-87-1P 443331-90-6P 443331-93-9P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
RACT
     (Reactant or reagent)
        (preparation of guanidine or guanidine pharmacophore-substituted
        oxodibenzazepineacetic acids as potential \alpha V\beta 3 receptor
        antagonists)
     326400-60-6 CAPLUS
RN
CN
     5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[4-(1H-benzimidazol-2-
     ylamino)phenyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo-, methyl
ester
     (9CI)
            (CA INDEX NAME)
```

PAGE 1-A

RN 326401-22-3 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[[[4-

[[[(phenylmethyl)amino]carbonyl]amino]phenyl]methyl]amino]ethyl]-,
methyl

ester (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 326408-08-6 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[6-(1H-benzimidazol-2-yl)-

3-

pyridinyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo-, methyl ester
(9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 326408-33-7 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[4-(1H-benzimidazol-2-yl)-2thienyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo-, methyl ester
(9CI)
(CA INDEX NAME)

RN 443331-29-1 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[(1H-benzimidazol-2-ylmethyl)amino]-2-oxoethyl]-6,11-dihydro-6-oxo-, methyl ester (9CI) (CA INDEX NAME)

RN 443331-31-5 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[4-(1H-benzimidazol-2-yl)phenyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo-, methyl ester (9CI)

(CA INDEX NAME)

ß

RN 443331-34-8 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[4-(1H-benzimidazol-2-yl)phenyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo-, methyl ester (9CI) (CA INDEX NAME)

RN 443331-37-1 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[2-[4-(1H-benzimidazol-2-yl)phenyl]ethyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo-, methyl ester (9CI)

(CA INDEX NAME)

RN 443331-42-8 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[3-(1H-benzimidazol-2-yl)phenyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo-, methyl ester (9CI) (CA INDEX NAME)

RN 443331-47-3 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[5-(1H-benzimidazol-2-yl)-2thienyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo-, methyl ester
(9CI)
(CA INDEX NAME)

IJ

RN 443331-50-8 CAPLUS

CN

2-

5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[4-(1H-benzimidazol-2-yl)-

thiazolyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo-, methyl ester (9CI) (CA INDEX NAME)

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IJ

443331-53-1 CAPLUS

RN

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-5-[2-[[[4-(1H-imidazo[4,5-b]pyridin-2-yl)-2-thienyl]methyl]amino]-2-oxoethyl]-6-oxo-, methyl ester (9CI) (CA INDEX NAME)

RN 443331-56-4 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-

[[[4-

[(2-pyridinylamino)methyl]-2-thienyl]methyl]amino]ethyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 443331-59-7 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[4-(aminoiminomethyl)-2-thienyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo-, methyl ester

(9CI) (CA INDEX NAME)

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PAGE 2-A

RN 443331-62-2 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[4-(5-chloro-1H-

benzimidazol-

2-yl)phenyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo-, methyl ester (9CI) (CA INDEX NAME)

RN 443331-65-5 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[4-(5,6-dimethyl-1H-benzimidazol-2-yl)phenyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo-, methyl ester (9CI) (CA INDEX NAME)

RN 443331-68-8 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[4[(aminoiminomethyl)amino]phenyl]methyl]amino]-2-oxoethyl]-6,11-dihydro6-

oxo-, methyl ester (9CI) (CA INDEX NAME)

RN 443331-87-1 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[4-(1H-benzimidazol-2-ylamino)butyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo-, methyl ester (9CI) (CA INDEX NAME)

RN 443331-90-6 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[5-(1H-benzimidazol-2-ylamino)pentyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo-, methyl ester (9CI)

(CA INDEX NAME)

RN 443331-93-9 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[trans-4-(1H-benzimidazol-2-

ylamino)cyclohexyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo-, methyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.

RE.CNT 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L7 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2005 ACS on STN
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AN 2001:115130 CAPLUS Full-text

DN 134:178474

TI Preparation of oxobenzazepinealkanoates and analogs as integrin receptor antagonists

IN Kling, Andreas; Geneste, Herve; Lange, Udo; Lauterbach, Arnulf; Graef, Claudia Isabella; Subkowski, Thomas; Holzenkamp, Uta; Mack, Helmut; Sadowski, Jens; Hornberger, Wilfried; Laux, Volker

PA BASF Aktiengesellschaft, Germany

SO PCT Int. Appl., 158 pp.

CODEN: PIXXD2

DT Patent

LA German

FAN.CNT 1

| T.LM. | PATENT NO.                     |                   |     |     | KIND     |                      | DATE |                   | APPLICATION NO. |                |     |          |          |          | DATE     |          |     |  |
|-------|--------------------------------|-------------------|-----|-----|----------|----------------------|------|-------------------|-----------------|----------------|-----|----------|----------|----------|----------|----------|-----|--|
| PI    | WO 2001010847<br>WO 2001010847 |                   |     |     |          | 20010215<br>20011101 |      | WO 2000-EP7440    |                 |                |     | 20000801 |          |          |          |          |     |  |
|       | W                              | : AE,             | AG. | AL. | AM.      | AT.                  | AU.  | AZ.               | BA.             | BB.            | BG. | BR.      | BY,      | BZ,      | CA,      | CH,      | CN, |  |
|       |                                |                   | CU, | •   | ,        | •                    | •    | •                 | •               | •              | •   |          |          | -        | -        | -        |     |  |
|       |                                | •                 | ID, |     |          |                      | •    | •                 | •               | •              |     | •        | -        | •        |          |          |     |  |
|       |                                | LU,               | LV, | MA, | MD,      | MG,                  | MK,  | MN,               | MW,             | MX,            | MZ, | NO,      | NZ,      | PL,      | PT,      | RO,      | RU, |  |
|       |                                |                   | SE, |     |          |                      |      |                   |                 |                |     |          |          |          |          |          |     |  |
|       |                                |                   | ZA, |     |          |                      |      |                   |                 |                |     |          |          |          |          |          |     |  |
|       | R                              | W: GH,            | GM, | KE, | LS,      | MW,                  | MZ,  | SD,               | SL,             | SZ,            | TZ, | UG,      | ZW,      | AT,      | BE,      | CH,      | CY, |  |
|       |                                | DE,               | DK, | ES, | FI,      | FR,                  | GB,  | GR,               | ΙE,             | IT,            | LU, | MC,      | NL,      | PT,      | SE,      | BF,      | ВJ, |  |
|       |                                | CF,               | CG, | CI, | CM,      | GΑ,                  | GN,  | GW,               | ML,             | MR,            | NE, | SN,      | TD,      | TG       |          |          |     |  |
|       | DE 19936780                    |                   |     | A1  |          | 2001                 | 0215 | DE 1999-19936780  |                 |                |     |          | 19990809 |          |          |          |     |  |
|       | CA 2379977                     |                   |     | AA  | 20010215 |                      |      | CA 2000-2379977   |                 |                |     |          | 20000801 |          |          |          |     |  |
|       | EP 1202988                     |                   |     |     | A2       | A2 20020508          |      |                   | EP 2000-958347  |                |     |          |          |          | 20000801 |          |     |  |
|       | P                              | : AT,             | BE, | CH, | DĖ,      | DK,                  | ES,  | FR,               | GB,             | GR,            | IT, | LI,      | LU,      | NL,      | SE,      | MC,      | PT, |  |
|       |                                | ΙE,               | SI, | LT, | LV,      | FI,                  | RO,  | MK,               | CY,             | AL             |     |          |          |          |          |          |     |  |
|       | BR 2000013265                  |                   |     |     | Α        |                      | 2002 | BR 2000-13265     |                 |                |     |          |          | 20000801 |          |          |     |  |
|       | TR 200200357                   |                   |     |     | Т2       |                      | 2002 | TR 2002-200200357 |                 |                |     |          |          | 20000801 |          |          |     |  |
|       | JP 2003506441                  |                   |     |     | Т2       |                      | 2003 | 0218              |                 | JP 2001-515313 |     |          |          |          |          | 20000801 |     |  |
|       | BG 106395                      |                   |     |     | Α        |                      | 2002 | 1229              |                 | BG 2002-106395 |     |          |          |          |          | 20020206 |     |  |
|       | NO 2002000644                  |                   |     |     | Α        |                      | 2002 |                   | NO 2002-644     |                |     |          |          |          | 20020208 |          |     |  |
| PRAI  | DE 1999-19936780               |                   |     |     | Α        |                      | 1999 | 0809              |                 |                |     |          |          |          |          |          |     |  |
|       | WO. 2000-EP7440                |                   |     |     | W        |                      | 2000 | 0801              |                 |                |     |          |          |          |          |          |     |  |
| os    | MARPA                          | MARPAT 134:178474 |     |     |          |                      |      |                   |                 |                |     |          |          |          |          |          |     |  |
| GI    |                                |                   |     |     |          |                      |      |                   |                 |                |     |          |          |          |          |          |     |  |

AB RZZ1R1 [I; R = group contg,  $\geq 1$  non-H H-bonding atom; R1 = CO2H, or group hydrolizable to CO2H; Z = e.g., (hetero)annelated 2-oxo-1-benzazepin-

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etc.] were prepared Thus, Me 11-methoxycarbonylmethyl-6- oxo-6,11-
     dihydro-5H-dibenz[b,e]azepine-5-acetate (preparation given) was amidated
     by N-(2-aminoethyl)pyridine-2-amine to give, after saponification, title
     compound II. Data for biol. activity of I were given.
     326398-79-2P 326398-84-9P 326398-90-7P
IT
     326399-01-3P 326399-07-9P 326399-11-5P
     326399-17-1P 326399-23-9P 326399-27-3P
     326399-31-9P 326399-36-4P 326399-42-2P
     326399-47-7P 326399-52-4P 326399-64-8P
     326399-69-3P 326399-73-9P 326399-78-4P
     326399-83-1P 326400-13-9P 326400-18-4P
     326400-23-1P 326400-28-6P 326400-32-2P
     326400-41-3P 326400-45-7P 326400-50-4P
     326400-55-9P 326400-60-6P 326400-65-1P
     326400-70-8P 326400-74-2P 326400-79-7P
     326400-84-4P 326400-88-8P 326400-94-6P
     326400-99-1P 326401-04-1P 326401-08-5P
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     326401-41-6P 326401-46-1P 326401-50-7P
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     326402-11-3P 326402-16-8P 326402-21-5P
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     326402-80-6P 326402-85-1P 326402-90-8P
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     326403-37-6P 326403-42-3P 326403-47-8P
     326403-61-6P 326403-66-1P 326403-71-8P
     326403-76-3P 326404-18-6P 326404-23-3P
     326404-27-7P 326404-31-3P 326404-36-8P
     326471-39-0P
     RL: BAC (Biological activity or effector, except adverse); BSU
(Biological
     study, unclassified); SPN (Synthetic preparation); THU (Therapeutic
     BIOL (Biological study); PREP (Preparation); USES (Uses)
        (preparation of oxobenzazepinealkanoates and analogs as integrin
receptor
        antagonists)
     326398-79-2 CAPLUS
RN
CN
     5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[[2-oxo-2-1]]]
(2 -
     pyridinylamino)ethyl]amino]ethyl]- (9CI) (CA INDEX NAME)
```

1,5-diyl; Z1 = bond, (un)substituted NHCH2, -OCH2, -alkylene, -CH:CH,

LH2-CO2H

RN 326398-84-9 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[4-(2-pyridinyl)-1-piperazinyl]ethyl]- (9CI) (CA INDEX NAME)

RN

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[6-(1H-benzimidazol-2-yl)-3-pyridinyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo-(9CI) (CA INDEX NAME)

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Сн2-со2н

RN 326399-01-3 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[2-[(4,5-dihydro-1H-imidazol-2-yl)amino]ethyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo-(9CI) (CA INDEX NAME)

Сн2-со2н

RN 326399-07-9 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[6-(4,5-dihydro-1H-imidazo]-2-

yl)-3-pyridinyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo-, monoacetate

(9CI) (CA INDEX NAME)

CM 1

CRN 326399-06-8 CMF C27 H25 N5 O4

Сн2-со2н

CM 2

CRN 64-19-7 CMF C2 H4 O2

о || но—С—Снз

RN 326399-11-5 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[[[1-

(2-pyridinyl)-4-piperidinyl]methyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 326399-17-1 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[(1H-benzimidazol-2-ylmethyl)amino]-2-oxoethyl]-6,11-dihydro-6-oxo-, monoacetate (9CI) (CFINDEX NAME)

CM 1

CRN 326399-16-0 CMF C26 H22 N4 O4

CM 2

CRN 64-19-7 CMF C2 H4 O2

RN 326399-23-9 CAPLUS

CN 5H-Dibenz[b,e] azepine-11-acetic acid, 6,11-dihydro-5-[2-[(1H-imidazo[4,5-

b]pyridin-2-ylmethyl)amino]-2-oxoethyl]-6-oxo-, monoacetate (9CI) (CA INDEX NAME)

CM 1

CRN 326399-22-8 CMF C25 H21 N5 O4

CM 2

CRN 64-19-7 CMF C2 H4 O2

RN\_ \_\_326399=27=3 \_\_CAPLUS \_\_\_\_\_

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[3-oxo-3-[[2-

(2-

pyridinylamino)ethyl]amino]propyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

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326399-31-9 CAPLUS RN

CN

5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[3-oxo-3-[4-(2-

pyridinyl)-1-piperazinyl]propyl]- (9CI) (CA INDEX NAME)

L<sub>H2-СО2Н</sub>

RN 326399-36-4 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[3-[[[4-(1H-benzimidazol-2-yl)-2-

thienyl]methyl]amino]-3-oxopropyl]-6,11-dihydro-6-oxo- (9CI) (CA INDEX NAME)

326399-42-2 CAPLUS RN

5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[4-CN[(2-

pyridinylamino)methyl]-1-piperidinyl]ethyl]-, monoacetate (9CI) (CA INDEX

NAME)

1 CM

CRN 326399-41-1 C29 H30 N4 O4 CMF

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CM

CRN 64-19-7 CMF C2 H4 O2

RN 326399-47-7 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[4-[(phenylmethyl)amino]carbonyl]-1-piperazinyl]ethyl]- (9CI) (CA INDEX NAME)

RN 326399-52-4 CAPLUS

CN 25H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[5-(1H-benzimidazol-2-yl)-

thienyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo- (9CI) (CA INDEX NAME)

RN 326399-64-8 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[4-(1H-benzimidazol-2-yl)-2-

thienyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo-, monoacetate (9CI) (CA INDEX NAME)

CM 1

CRN 326399-63-7 CMF C30 H24 N4 O4 S

CM 2

CRN 64-19-7 CMF C2 H4 O2

RN

326399-69-3 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-5-[2-[[[4-(1H-imidazo[4,5-b]pyridin-2-yl)-2-thienyl]methyl]amino]-2-oxoethyl]-6-oxo-(9CI) (CA INDEX NAME)

RN 326399-73-9 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[4-(1H-benzimidazol-2-yl)phenyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo-, monohydrochloride

(9CI) (CA INDEX NAME)

СH2-СО2Н

HC1

326399-78-4 CAPLUS RN

5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[4-(1H-benzimidazol-2-yl)-

CN 2-

CN

thiazolyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo- (9CI) (CA INDEX NAME)

RN 326399-83-1 CAPLUS

5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[4-(1H-benzimidazol-2-

yl)phenyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo- (9CI) (CA INDEX NAME)

RN 326400-13-9 CAPLUS

CN 5H-Dibenz[b,e] azepine-11-acetic acid, 6,11-dihydro-5-[2-[[3-(1H-imidazol-2-[2-[[3-(1H-imidazol-2-[2-[3-(1H-imidazol-2-[3-(1H-imida

ylamino)-3-oxopropyl]amino]-2-oxoethyl]-6-oxo- (9CI) (CA INDEX NAME)

RN 326400-18-4 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[4-[[[(phenylmethyl)amino]carbonyl]amino]methyl]-1-piperidinyl]ethyl]-(9CI)

(CA INDEX NAME)

RN 326400-23-1 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[3-oxo-3-[[1-

(2-pyridinyl)-4-piperidinyl]methyl]amino]propyl]- (9CI) (CA INDEX NAME)

RN 326400-32-2 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[3-[[[5-(1H-benzimidazol-2-yl)-2-thienyl]methyl]aminol-3-ovopropyll-6 11-dibydro-6-ovo- (9CI) (CA INDEX

thienyl]methyl]amino]-3-oxopropyl]-6,11-dihydro-6-oxo- (9CI) (CA INDEX NAME)

 $L_{\text{CH}_2-\text{CO}_2\text{H}}$ 

Сн2—со2н

RN 326400-45-7 CAPLUS CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[[[4-

сн<sub>2</sub>— со<sub>2</sub>н

RN 326400-50-4 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[4-(2-

pyridinylamino)-1-piperidinyl]ethyl]- (9CI) (CA INDEX NAME)

RN 326400-55-9 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[4-(1H-benzimidazol-2-ylamino)phenyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 326400-60-6 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[4-(1H-benzimidazol-2-ylamino)phenyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo-, methyl ester

(9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 326400-65-1 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[5-(1H-benzimidazol-2-ylamino)pentyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo- (9CI) (CA INDEX NAME)

RN

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[4-(1H-benzimidazol-2-ylamino)butyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo-(9CI) (CA INDEX NAME)

RN 326400-74-2 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[[[3-

[[[(phenylmethyl)amino]carbonyl]amino]phenyl]methyl]amino]ethyl]- (9CI)
(CA INDEX NAME)

RN 326400-79-7 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[4-[(1H-benzimidazol-2-ylamino)methyl]-1-piperidinyl]-2-oxoethyl]-6,11-dihydro-6-oxo- (9CI)

(CA INDEX NAME)

NAME)

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE RN 326400-94-6 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[2-[(aminoiminomethyl)amino]-4-thiazolyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 326400-93-5 CMF C23 H22 N6 O4 S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 326400-99-1 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[2[(aminoiminomethyl)amino]5-thiazolyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo- (9CI) (CA
INDEX
NAME)

RN 326401-04-1 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[2-[4-(1H-benzimidazol-2-yl)phenyl]ethyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo- (9CI) (CA INDEX NAME)

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PAGE 1-A

PAGE 2-A

CH<sub>2</sub>.

RN 326401-13-2 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-5=[2-[methyl[2-(2-pyridinylamino)ethyl]amino]-2-oxoethyl]-6-oxo- (9CI) (CA INDEX NAME)

L Сн2-со2н

CH2-CO2H

RN 326401-32-5 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[4[(aminoiminomethyl)amino]phenyl]methyl]amino]-2-oxoethyl]-6,11-dihydro6oxo-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 326401-31-4 CMF C26 H25 N5 O4

Сн2-со2н

CM

CRN 76-05-1 CMF C2 H F3 O2

326401-36-9 CAPLUS RN

5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[4-(5-chloro-1H-CN

benzimidazol-

2-yl)phenyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo- (9CI) INDEX

NAME)

Сн2-со2н

RN 326401-41-6 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[4-(5,6-dimethyl-1H-benzimidazol-2-yl)phenyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo-(9CI) (CA INDEX NAME)

PAGE 1-A

CH2-CO2H

RN 326401-46-1 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[[3-(2-pyridinylamino)propyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 326401-50-7 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[4-[2-(2-pyridinylamino)ethyl]-1-piperidinyl]ethyl]-, methyl ester (9CI) (CA INDEX NAME)

\

RN 326401-54-1 CAPLUS

5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[4-CN [2-

(2-pyridinylamino)ethyl]-1-piperidinyl]ethyl]- (9CI) (CA INDEX NAME)

RN 326401-59-6 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[3-

[2- (2-pyridinylamino)ethyl]-1-pyrrolidinyl]ethyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 326401-64-3 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[3-[2-(2-pyridinylamino)ethyl]-1-pyrrolidinyl]ethyl]- (9CI) (CA INDEX NAME)

СН2-СО2Н

Сн2-со2н

RN 326401-82-5 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[5-[[[(phenylmethyl)amino]carbonyl]amino]pentyl]- (9CI) (CA INDEX NAME)

RN 326401-92-7 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-[[4-[[(phenylmethyl)amino]carbonyl]amino]phenyl]methoxy]ethyl]- (9CI) (CA INDEX NAME)

Сн2-со2н

RN 326401-97-2 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[4-[4-[(phenylmethyl)amino]carbonyl]amino]phenyl]butyl]- (9CI) (CA INDEX NAME)

326402-06-6 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-5-[2-[[3-(4-methyl-

1H-

RN 326402-11-3 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-5-[2-[[3-(4-methyl-1-piperazinyl)propyl]amino]-2-oxoethyl]-6-oxo- (9CI) (CA INDEX NAME)

RN 326402-16-8 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[(3-pyridinylmethyl)amino]ethyl]- (9CI) (CA INDEX NAME)

RN 326402-21-5 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-5-[2-[[3-(1H-imidazol-1-yl)propyl]amino]-2-oxoethyl]-6-oxo-(9CI) (CA INDEX NAME)

RN 326402-26-0 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-5-[2-[[1-methyl-2-(4-morpholinyl)ethyl]amino]-2-oxoethyl]-6-oxo- (9CI) (CA INDEX NAME)

RN 326402-31-7 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[(1-ethyl-2-pyrrolidinyl)methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo- (9CI) (CA INDEX NAME)

RN 326402-35-1 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[4-(4-pyridinylmethyl)-1-piperazinyl]ethyl]- (9CI) (CA INDEX NAME)

 $L_{\rm H2-CO2H}$ 

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RN 326402-44-2 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[4-[2-(diethylamino)ethyl]-1-piperazinyl]-2-oxoethyl]-6,11-dihydro-6-oxo- (9CI) (CA INDEX NAME)

RN 326402-48-6 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-5-[2-[4-[2-(4-morpholinyl)ethyl]-1-piperazinyl]-2-oxoethyl]-6-oxo- (9CI) (CA INDEX NAME)

RN 326402-52-2 CAPLUS

(2-

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[4-

pyrimidinyl)-1-piperazinyl]ethyl]- (9CI) (CA INDEX NAME)

RN 326402-57-7 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[(2-pyridinylmethyl)amino]ethyl]- (9CI) (CA INDEX NAME)

RN 326402-62-4 CAPLUS

CN 5H-Dibenz[b,ė]azepine-11-acetic acid, 6,11-dihydro-5-[2-[[2-(4-morpholinyl)ethyl]amino]-2-oxoethyl]-6-oxo- (9CI) (CA INDEX NAME)

RN 326402-66-8 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[3-(dibutylamino)propyl]amino]2-oxoethyl]-6,11-dihydro-6-oxo- (9CI) (CA INDEX NAME)

RN 326402-71-5 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[4-(4-pyridinyl)-1-piperazinyl]ethyl]- (9CI) (CA INDEX NAME)

RN 326402-76-0 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-5-[2-[4-[3-(4-morpholinyl)propyl]-1-piperazinyl]-2-oxoethyl]-6-oxo- (9CI) (CA INDEX NAME)

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Сн2-со2н

RN 326402-80-6 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-5-[2-[[3-(2-methyl-

1H-

imidazol-1-yl)propyl]amino]-2-oxoethyl]-6-oxo- (9CI) (CA INDEX NAME)

RN 326402-85-1 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[(4-pyridinylmethyl)amino]ethyl]- (9CI) (CA INDEX NAME)

RN 326402-90-8 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-5-[2-[(1-methyl-4-piperidinyl)amino]-2-oxoethyl]-6-oxo- (9CI) (CA INDEX NAME)

RN 326402-94-2 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[[2-(1-piperidinyl)ethyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 326402-99-7 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[4-[3-(1-pyrrolidinyl)propyl]-1-piperazinyl]ethyl]- (9CI) (CA INDEX NAME)

 $c_{\rm H2-CO2H}$ 

RN 326403-04-7 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[4-[2-(dimethylamino)ethyl]1piperazinyl]-2-oxoethyl]-6,11-dihydro-6-oxo- (9CI) (CA INDEX NAME)

RN 326403-08-1 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[4-[3-(dimethylamino)propyl]-

1piperazinyl]-2-oxoethyl]-6,11-dihydro-6-oxo- (9CI) (CA INDEX NAME)

RN 326403-13-8 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[4-[2-(dipropylamino)ethyl]-1piperazinyl]-2-oxoethyl]-6,11-dihydro-6-oxo- (9CI) (CA INDEX NAME)

RN 326403-18-3 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[4-[2-(1-piperidinyl)ethyl]-1-piperazinyl]ethyl]- (9CI) (CA INDEX NAME)

RN 326403-22-9 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[4-[3-(dipropylamino)propyl]1piperazinyl]-2-oxoethyl]-6,11-dihydro-6-oxo- (9CI) (CA INDEX NAME)

RN 326403-28-5 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[4-(dibutylamino)butyl]amino]2-oxoethyl]-6,11-dihydro-6-oxo- (9CI) (CA INDEX NAME)

RN 326403-32-1 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[4-[2-oxo-2-(1-pyrrolidinyl)ethyl]-1-piperazinyl]ethyl]- (9CI) (CA INDEX NAME)

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RN 326403-37-6 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[3-(diethylamino)propyl]amino]2-oxoethyl]-6,11-dihydro-6-oxo- (9CI) (CA INDEX NAME)

RN 326403-42-3 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[2-(dimethylamino)ethyl]amino]2-oxoethyl]-6,11-dihydro-6-oxo-(9CI) (CA INDEX NAME)

$$\begin{array}{c} \begin{array}{c} \begin{array}{c} \begin{array}{c} \begin{array}{c} \begin{array}{c} \begin{array}{c} \\ \end{array}\\ \end{array}\\ \end{array}\\ \begin{array}{c} \\ \end{array}\\ \end{array}\\ \begin{array}{c} \\ \end{array}\\ \begin{array}{c} \\ \end{array}\\ \begin{array}{c} \\ \end{array}\\ \end{array}\\ \begin{array}{c} \\ \end{array}\\ \begin{array}{c} \\ \end{array}\\ \begin{array}{c} \\ \end{array}\\ \end{array}$$

RN 326403-47-8 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[4-(dimethylamino)butyl]amino]2-oxoethyl]-6,11-dihydro-6-oxo- (9CI) (CA INDEX NAME)

RN 326403-61-6 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-propanoic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[[[4-[[(phenylmethyl)amino]carbonyl]amino]phenyl]methyl]amino]ethyl]-, methyl ester (9CI) (CA INDEX NAME)

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RN 326403-66-1 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-propanoic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[[[4-[[(phenylmethyl)amino]carbonyl]amino]phenyl]methyl]amino]ethyl]-(9CI) (CA INDEX NAME)

Сн2-Сн2-Со2н

 $L_{\text{H}_2-\text{CH}_2}$  — OMe

RN 326403-76-3 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-propanoic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-

[[2- (2-pyridinylamino)ethyl]amino]ethyl]-, monosodium salt (9CI) (CA INDEX NAME)

Сн2-сн2-со2н

Na

RN 326404-18-6 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[[4-[[[[4-(1H-benzimidazol-2-yl)phenyl]methyl]amino]carbonyl]-2-thiazolyl]methyl]-6,11-dihydro-6-oxo-(9CI) (CA INDEX NAME)

RN 326404-23-3 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[[4-[[4-[(2-pyridinylamino)methyl]-1-piperidinyl]carbonyl]-2-thiazolyl]methyl](9CI)

(CA INDEX NAME)

RN 326404-27-7 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[[4-[[[[4-[[(phenylmethyl)amino]carbonyl]amino]phenyl]methyl]amino]carbonyl]-2-thiazolyl]methyl]- (9CI) (CA INDEX NAME)

326404-31-3 CAPLUS

RN

CN

5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[[4-[[[[4-

RN 326404-36-8 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[[4-[[[4[(2pyridinylamino)methyl]-2-thienyl]methyl]amino]carbonyl]-2-

pyridinylamino)methyl]-2-thienyl]methyl]amino]carbonyl]-2thiazolyl]methyl]- (9CI) (CA INDEX NAME)

RN 326471-39-0 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[4-(aminoiminomethyl)-2-thienyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo-, monoacetate (9CI) (CA INDEX NAME)

CM 1

CRN 326471-38-9 CMF C24 H22 N4 O4 S

CM 2

CRN 64-19-7 CMF C2 H4 O2

HO-C-CH3

```
IT
    326407-99-2P 326408-04-2P 326408-08-6P
    326408-13-3P 326408-23-5P 326408-28-0P
    326408-33-7P 326408-41-7P 326408-46-2P
    326408-54-2P 326410-02-0P 326410-07-5P
    RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
RACT
     (Reactant or reagent)
        (preparation of oxobenzazepinealkanoates and analogs as integrin
receptor
        antagonists)
RN
     326407-99-2 CAPLUS
     5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[[2-
CN
(2-
     pyridinylamino)ethyl]amino]ethyl]-, methyl ester (9CI) (CA INDEX NAME)
```

RN 326408-04-2 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[4-(2-pyridinyl)-1-piperazinyl]ethyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 326408-08-6 CAPLUS

3--

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[6-(1H-benzimidazol-2-yl)-

pyridinyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo-, methyl ester
(9CI) (CA INDEX NAME)

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CH2—C—OMe

RN 326408-13-3 CAPLUS

CN 5H-Dibenz[b,e]azepine-ll-acetic acid, 5-[2-[4-[(1,1-dimethylethoxy)carbonyl]-1-piperazinyl]-2-oxoethyl]-6,11-dihydro-6-oxo-, methyl ester (9CI) (CA INDEX NAME)

RN 326408-23-5 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[5-(aminothioxomethyl)-2-thienyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo-, methyl ester (9CI)

(CA INDEX NAME)

RN 326408-28-0 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[5-(aminoiminomethyl)-2-thienyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo-, methyl ester (9CI)

(CA INDEX NAME)

RN 326408-33-7 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 5-[2-[[[4-(1H-benzimidazol-2-yl)-2thienyl]methyl]amino]-2-oxoethyl]-6,11-dihydro-6-oxo-, methyl ester
(9CI)
(CA INDEX NAME)

RN 326408-41-7 CAPLUS
CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-5-[2-[[3-(1H-imidazol-2-ylamino)-3-oxopropyl]amino]-2-oxoethyl]-6-oxo-, methyl ester (9CI) (CA INDEX NAME)

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RN 326408-46-2 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-5-[2-[[[5-[(hydroxyamino)iminomethyl]-2-thienyl]methyl]amino]-2-oxoethyl]-6-oxo-, methyl ester (9CI) (CA INDEX NAME)

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RN 326408-54-2 CAPLUS

5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[5-[[[(phenylmethyl)amino]carbonyl]amino]pentyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 326410-02-0 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-(1-piperazinyl)ethyl]-, methyl ester, mono(trifluoroacetate) (9CI) (CA INDEX

NAME)

CM 1

CRN 326410-01-9 CMF C23 H25 N3 O4

$$\begin{array}{c} H \\ N \\ C = 0 \\ CH2 \\ N \\ CH2-C-OMe \\ 0 \\ \end{array}$$

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 326410-07-5 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-5-[2-oxo-2-[4-[[(phenylmethyl)amino]carbonyl]-1-piperazinyl]ethyl]-, methyl ester (9CI)

(CA INDEX NAME)

- L7 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2005 ACS on STN
- AN 1989:632774 CAPLUS Full-text
- DN 111:232774
- TI Preparation of tricyclic lactams and analogs as muscarinic antagonists
- IN Turconi, Marco; Donetti, Arturo; Cereda, Enzo; Quintero, Myrna Gil; Schiavi, Giovanni Battista; Micheletti, Rosamaria
- PA Istituto De Angeli S.p.A., Italy
- SO Eur. Pat. Appl., 46 pp.

CODEN: EPXXDW

DT Patent

LA English

FAN.CNT 1

|      | PATENT NO. |      |      |     | KIND |            | DATE |       | API  | APPLICATION NO. |        |        |       | DATE |       |     |
|------|------------|------|------|-----|------|------------|------|-------|------|-----------------|--------|--------|-------|------|-------|-----|
|      |            |      |      |     |      |            |      |       |      |                 |        |        |       |      |       |     |
| PI   | EP         | 3094 | 22   |     |      | A2         |      | 1989  | 0329 | EP              | 1988-  | -83037 | 4     |      | 19880 | 919 |
|      | EP 309422  |      |      | A3  |      | 19900110   |      |       |      |                 |        |        |       |      |       |     |
|      |            | R:   | ΑT,  | BE, | CH,  | DE,        | ES   | , FR, | GB,  | GR, I           | r, LI, | LU,    | NL, S | EΕ   |       |     |
|      | DD         | 2826 | 89   |     |      | A5         |      | 1990  | 0919 | DD              | 1988-  | -31983 | 1     |      | 19880 | 915 |
|      | DK         | 8805 | 226  |     |      | Α          |      | 1989  | 0322 | DK              | 1988-  | -5226  |       |      | 19880 | 920 |
|      | FI         | 8804 | 305  |     |      | Α          |      | 1989  | 0322 | FI              | 1988-  | -4305  |       |      | 19880 | 920 |
|      | NO         | 8804 | 174  |     |      | Α          |      | 1989  | 0322 | NO              | 1988-  | -4174  |       |      | 19880 | 920 |
|      | JP         | 0113 | 2567 |     |      | A2         |      | 1989  | 0525 | JP              | 1988-  | -23617 | 8     |      | 19880 | 920 |
|      | AU         | 8822 | 380  |     |      | <b>A</b> 1 |      | 1989  | 0323 | AU              | 1988-  | -22380 | )     |      | 19880 | 921 |
| PRAI | IT         | 1987 | -219 | 78  |      | Α          |      | 1987  | 0921 |                 |        |        |       |      |       |     |
| PRAI | IT         | 1987 | -219 | 78  |      | Α          |      | 1987  | 0921 |                 |        |        |       |      |       |     |

- OS MARPAT 111:232774
- GI For diagram(s), see printed CA Issue.
- Title compds. I [R = H, halo; X = N, CH; W = NHCO, CH: CH: CH2)2, O, S; AB R1 = H, C1-4 alkyl; n = 0, 1; Y = S, CH; A = C, N; B = CH when  $A \neq N$ , CO2, CO, CH2; m = 0-3; Z = NH, CO, CO2, CH, bond; p,q = 0, 1; Q = 0(homo)piperazinyl, piperidinyl, tropyl, tetrahydroprimidinyl, the above groups may be substituted by a C1-4 alkyl or an amino; R = CR2:NR3; R2 = H, C1-4 alkyl, (C1-4 alkyl- or Ph-substituted) amino; R3 = C1-8 alkyl, H (provided that the bond of QR is a C-C bond or AB = C:CH); R2R3 = atoms to form a 5-membered ring] are prepared for treatment of motility disorders of the gastrointestinal or urogenital tract and peptic ulcer disorders. A mixture of 5,10-dihydro-5-[2-piperazin-1-yl)acetyl]-11Hdibenzo[b,e][1,4]- diazepin-11-one and H2NC(:NH)SMe.H2SO4 in EtOH was refluxed to give the 4-quanylpiperazinyl analog isolated as its 2 HCl salt. The latter salt showed a dissociation constant (kD) of 6 nM for displacement of 3H-pirenzepine from cerebral cortex homogenate of rats. Tablets were formulated containing I 20, lactose 247, cornstarch 30, and Mg stearate 3 mg.

## 1T 122860-50-8P 122860-58-6P 122860-66-6P 122860-68-8P 122882-85-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and reaction of, in preparation of muscarinic antagonists)

- RN 122860-50-8 CAPLUS
- CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-, 1-[imino(nitroamino)methyl]-4-piperidinyl ester (9CI) (CA INDEX NAME)

RN 122860-58-6 CAPLUS

CN Acetic acid, (5,6-dihydro-6-oxo-11H-dibenz[b,e]azepin-11-ylidene)-, 1-[imino(nitroamino)methyl]-4-piperidinyl ester (9CI) (CA INDEX NAME)

RN 122860-66-6 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-carboxylic acid, 6,11-dihydro-6-oxo-, 1-[imino(nitroamino)methyl]-4-piperidinyl ester (9CI) (CA INDEX NAME)

RN - 122860-68-8 - CAPLUS - - - - - -

CN 5H-Dibenz[b,e]azepine-11-carboxylic acid, 6,11-dihydro-6-oxo-,

1,4,5,6-tetrahydro-2-(nitroamino)-5-pyrimidinyl ester (9CI) (CA INDEX NAME)

RN 122882-85-3 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-carboxylic acid, 6,11-dihydro-6-oxo-, 1-[imino(nitroamino)methyl]-3-piperidinyl ester (9CI) (CA INDEX NAME)

1T 122882-58-0P 122882-61-5P 122882-62-6P 122882-63-7P 122882-64-8P 122882-66-0P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of, as muscarinic antagonist)

RN 122882-58-0 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-acetic acid, 6,11-dihydro-6-oxo-, 1-(aminoiminomethyl)-4-piperidinyl ester, monoformate (9CI) (CA INDEX NAME)

CM 1

CRN 122882-57-9 CMF C22 H24 N4 O3

CM 2

CRN 64-18-6 CMF C H2 O2

о== СН-ОН

RN 122882-61-5 CAPLUS

CN Acetic acid, (5,6-dihydro-6-oxo-11H-dibenz[b,e]azepin-11-ylidene)-, 1-(aminoiminomethyl)-4-piperidinyl ester, monohydrochloride (9CI) (CA INDEX NAME)

RN 122882-62-6 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-carboxylic acid, 6,11-dihydro-6-oxo-, 1-(aminoiminomethyl)-4-piperidinyl ester, monohydrochloride (9CI) (CA INDEX NAME)

RN 122882-63-7 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-carboxylic acid, 6,11-dihydro-6-oxo-, 1-(aminoiminomethyl)-3-piperidinyl ester, monohydrochloride (9CI) (CA INDEX NAME)

## HCl

RN 122882-64-8 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-carboxylic acid, 6,11-dihydro-6-oxo-, 2-amino-1,4,5,6-tetrahydro-5-pyrimidinyl ester, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 122882-66-0 CAPLUS
CN 5H-Dibenz[b,e]azepine-ll-carboxylic acid, 6,11-dihydro-6-oxo-,
[1-(aminoiminomethyl)-4-piperidinyl]methyl ester, monoformate (9CI) (CA INDEX NAME)

CM 1

CRN 122882-65-9 CMF C22 H24 N4 O3

CM 2

CRN 64-18-6 CMF C H2 O2

O == CH - OH

L7 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1987:4907 CAPLUS Full-text

DN 106:4907

TI Preparation of morphanthridine analogs as pharmaceuticals

IN Senda, Shigeo; Ueda, Takashi; Nakagawa, Kazuyuki

PA Otsuka Pharmaceutical Co., Ltd., Japan

SO Jpn. Kokai Tokkyo Koho, 21 pp.

CODEN: JKXXAF

DT Patent

LA Japanese

FAN. CNT 1

| PATENT NO.        | KIND | DATE     | DATE         |          |  |
|-------------------|------|----------|--------------|----------|--|
|                   |      |          |              |          |  |
| PI JP 61167663    | A2   | 19860729 | JP 1985-7854 | 19850118 |  |
| JP 06065664       | B4   | 19940824 |              |          |  |
| PRAI JP 1985-7854 |      | 19850118 |              |          |  |
| GI                | •    |          |              |          |  |

AB Analogs of morphanthridine (I) are prepared and are useful in the treatment of arrhythmia, inflammation, diuresis, and ulcer. Thus, I was prepared by treating 5-methyl-l1-carboxy-6-oxomorphanthridine first with thionyl chloride and then with diethylaminoethanol. Thirty-four I analogs were prepared The inhibitory actions of I analogs on gastric acid secretion were demonstrated. No other pharmacol. studies were described.

## IT 105671-18-9P 105671-33-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of, as pharmaceutical)

RN 105671-18-9 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-carboxylic acid, 5-[2-(dimethylamino)-2-oxoethyl]-6,11-dihydro-6-oxo-, 2-(diethylamino)ethyl ester (9CI) (CA INDEX NAME)

RN 105671-33-8 CAPLUS

CN 5H-Dibenz[b,e]azepine-11-carboxylic acid, 5-[2-(dimethylamino)-2-oxoethyl]-6,11-dihydro-6-oxo- (9CI) (CA INDEX NAME)

$$\begin{array}{c} O \\ CH_2 - C - NMe_2 \\ \hline \\ CO_2H \end{array}$$

L7 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1984:103199 CAPLUS Full-text

DN 100:103199

TI 5,6-Dihydro-11-alkylenemorphanthridin-6-ones and a drug containing them

IN Steiner, Gerd; Friedrich, Ludwig; Lenke, Dieter

PA BASF A.-G., Fed. Rep. Ger.

SO Ger. Offen., 18 pp.

CODEN: GWXXBX

DT Patent

LA German

FAN.CNT 1

| r AIV.   | PATENT NO.  | KIND                    | DATE  | APPLICATION NO.                                     | DATE                             |
|----------|---|-------------------------|---|---|----------------------------------|
| ΡΙ       | DE 3212794<br>CA 1215046<br>EP 91057<br>EP 91057      | A1<br>A1<br>A2<br>A3    | 19831013<br>19861209<br>19831012<br>19840502      | DE 1982-3212794<br>CA 1983-424134<br>EP 1983-103054 | 19820406<br>19830322<br>19830328 |
|          | EP 91057<br>R: AT, BE, CH,<br>AT 20345<br>JP 58192871 | B1<br>DE, FF<br>E<br>A2 | 19860611<br>R, GB, IT, L1<br>19860615<br>19831110 | I, NL, SE<br>AT 1983-103054<br>JP 1983-58804        | 19830328<br>19830405             |
| PRAI     | US 4477451<br>DE 1982-3212794<br>EP 1983-103054       | A<br>A<br>A             | 19841016<br>19820406<br>19830328                  | US 1983-482004                                      | 19830405                         |
| OS<br>GT | CASREACT 100:103199                                   |                         | •   |   |                                  |

AB Morphanthridinones I [R1,R2 = H, halo, C1-3 alkyl, CF3; R3 = C2-4 aminoalkyl, N (un)substituted with C1-3 alkyl or may complete a 5- to 7-membered saturated ring, optionally having N, O, or S atom as further heteroatom or CO group; R4 = H; R3R4 complete a 5- to 7-membered ring, C1-3 alkyl (un)substituted, optionally having CH2 or (CH2)2 bridge or a N atom alkyl (un)substituted or N-oxide], useful in treating gastric or duodenal ulcers (no data), were prepared A mixture of cis- and trans-11-(carbomethoxymethylene)-5,6-dihydromorphanthridin-6-one was saponified with 10% aqueous alc. NaOH to give 94% of the free acids which were converted to 99% of the acid chlorides with SOC12. Esterification of the acid chlorides with 4-(2-hydroxyethyl)morpholine gave 66% cis- and trans-II.

## IT 88695-66-3

RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation as ulcer inhibitor)

RN 88695-66-3 CAPLUS

CN Acetic acid, (5,6-dihydro-6-oxo-11H-dibenz[b,e]azepin-11-ylidene)-,

8-methyl-8-azabicyclo[3.2.1]oct-3-yl ester (9CI) (CA INDEX NAME)

=> d 11; d 12; d his; log y L1 HAS NO ANSWERS

т.1

STR

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

Structure attributes must be viewed using STN Express query preparation.

L2 HAS NO ANSWERS

L2

STR

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

Structure attributes must be viewed using STN Express query preparation.

(FILE 'STNGUIDE' ENTERED AT 18:52:38 ON 06 JAN 2005)
DEL HIS Y

FILE 'REGISTRY' ENTERED AT 18:59:17 ON 06 JAN 2005

L1 STRUCTURE UPLOADED

L2 STRUCTURE UPLOADED

L3 1 S L1

L4 4 S L2

L5 4 S L1 OR L2

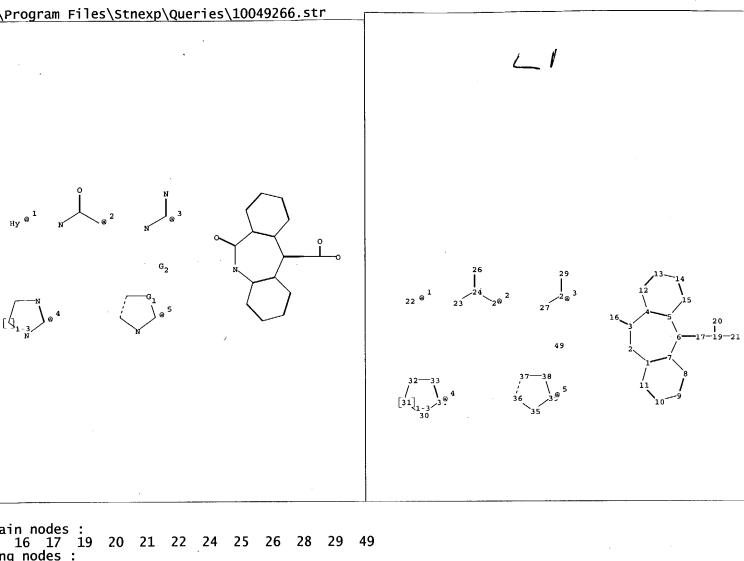
L6 193 S L1 OR L2 FUL

FILE 'CAPLUS' ENTERED AT 19:02:50 ON 06 JAN 2005

L7 6 S L6

| COST IN U.S. DOLLARS                       | SINCE FILE | TOTAL   |
|--|------------|---------|
|  | ENTRY      | SESSION |
| FULL ESTIMATED COST                        | 30.09      | 280.76  |
|  |            |         |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE | TOTAL   |
|  | ENTRY      | SESSION |
| CA SUBSCRIBER PRICE                        | -4.38      | -4.38   |

STN INTERNATIONAL LOGOFF AT 19:03:39 ON 06 JAN 2005



```
ng nodes:

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 30 31 32 33 34 35 36 37 38 39 ng/chain nodes:

23 27 ain bonds:

3-16 6-17 17-19 19-20 19-21 23-24 24-25 24-26 27-28 28-29 ng bonds:

1-2 1-7 1-11 2-3 3-4 4-5 4-12 5-6 5-15 6-7 7-8 8-9 9-10 10-11 12-13 13-14 14-15 30-31 30-34 31-32 32-33 33-34 35-36 35-39 36-37 37-38 38-39 act/norm bonds:

1-2 2-3 3-4 3-16 5-6 6-7 6-17 17-19 19-20 19-21 23-24 24-25 24-26 27-28 28-29 30-31 30-34 31-32 32-33 33-34 35-36 35-39 36-37 37-38 38-39 rmalized bonds:

1-7 1-11 4-5 4-12 5-15 7-8 8-9 9-10 10-11 12-13 13-14 14-15
```

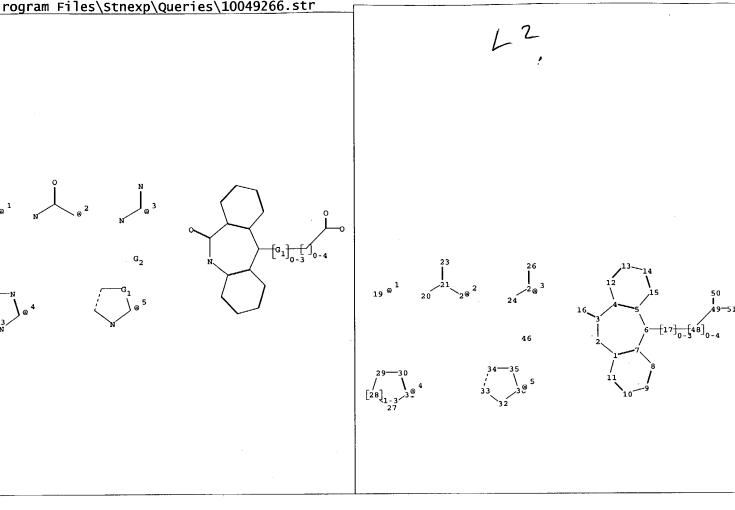
:[\*1],[\*2],[\*3],[\*4],[\*5]

tch level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 17:CLASS 19:CLASS 20:CLASS 21:CLASS
22:Atom 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:Atom
31:Atom 32:Atom 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 49:CLASS
neric attributes:
22:

Saturation : Unsaturated
Number of Carbon Atoms : less than 7
Number of Hetero Atoms : less than 2
Type of Ring System : Monocyclic

ement Count :

:C,0



```
n nodes:
16 17 19 21 22 23 25 26 46 48 49 50 51
3 nodes:
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 27 28 29 30 31 32 33 34 35 36
3/chain nodes:
20 24
n bonds:
3-16 6-17 17-48 20-21 21-22 21-23 24-25 25-26 48-49 49-50 49-51
3 bonds:
1-2 1-7 1-11 2-3 3-4 4-5 4-12 5-6 5-15 6-7 7-8 8-9 9-10 10-11 12-13 13-14
14-15 27-28 27-31 28-29 29-30 30-31 32-33 32-36 33-34 34-35 35-36
21/chorm bonds:
1-2 2-3 3-4 3-16 5-6 6-7 6-17 17-48 20-21 21-22 21-23 24-25 25-26 27-28 27-31
28-29 29-30 30-31 32-33 32-36 33-34 34-35 35-36 48-49 49-50 49-51
malized bonds:
1-7 1-11 4-5 4-12 5-15 7-8 8-9 9-10 10-11 12-13 13-14 14-15
```

[\*1],[\*2],[\*3],[\*4],[\*5]

th level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 17:Atom 19:Atom 20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom 32:Atom 33:Atom 34:Atom 35:Atom 36:Atom 46:CLASS 48:CLASS 49:CLASS 50:CLASS 51:CLASS 51

Saturation : Unsaturated
Number of Carbon Atoms : less than 7
Number of Hetero Atoms : less than 2
Type of Ring System : Monocyclic